

Template Constrained Macrocyclic Peptides Prepared from Native Unprotected Precursors

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Supporting Information

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General:

Unless stated otherwise, reactions were performed under an argon atmosphere in flame-dried glassware. Tetrahydrofuran (THF) was deoxygenated and dried by passing through an activated alumina solvent drying system. Anhydrous *N,N*-dimethylformamide (EMD DriSolv®) was used without further purification.

Purification of acidolysis products employed an Agilent 1100/1200 HPLC system equipped with G1361A preparative pumps, a G1314A autosampler, a G1314A VWD, and a G1364B automated fraction collector. Analytical HPLC was performed using the same system, but with a G1312A binary pump. Mass spectra were recorded using an Agilent 6130 LC/MS system equipped with an ESI source.

NMR methods:

NMR spectra were recorded on BrukerAvance (500 or 600 MHz) spectrometers. Data for ^1H NMR spectra are reported as: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration), and are referenced to a residual DMSO-*d*₆ (2.50ppm). ^{13}C resonances are reported in terms of chemical shift (δ ppm) as referenced to DMSO-*d*₆ (39.52 ppm). For mass-limited samples, solvent magnetic susceptibility matched Shigemi tubes were used with a sample volume of ~ 300 μL . Optimization of on-axis shims was accomplished using the TopShim automated tool within Bruker Topspin™ 2.1. Optimization of off-axis shims was performed manually,¹ or with TopShim3D in the case of samples containing H₂O. ^1H 90° transmitter pulse lengths were calibrated by back calculation from the 360° null.² The pulse width or power level for soft pulses and shaped pulses were calculated using the Shape Tool within TopSpin™ 2.1.

COSY spectra were recorded using a phase sensitive, gradient enhanced double-quantum-filtered experiment,³ or magnitude mode gradient enhanced experiment with presaturation using the States-TPPI method. Data were typically recorded as a matrix of 2048 x 512 complex points and 2 transients per increment. Data were apodized with a $\pi/3$ -shifted sine-bell in the F1 dimension truncated at 10%, and with an untruncated $\pi/3$ -shifted sine-bell in the F2 dimension. Zero filling was applied in F2 to give a symmetrical matrix of 4K x 4K real points following mirror image linear prediction in F1 (64 coefficients) to 256 points.

TOCSY spectra were recorded using a phase sensitive experiment implementing preservation of equivalent pathways.⁴ A 60ms DIPSI-2 or MLEV pulse train was used for homonuclear Hartman-Hahn transfer.⁵ Data were typically recorded as a matrix of 2048 x 256 complex points and 2 or 8 transients per increment. Data were apodized with a $\pi/3$ -shifted squared sine-bell in the F1 dimension truncated at 10%, and with an untruncated $\pi/2$ -shifted squared sine-bell in the F2 dimension. Zero filling was applied in F2 to give a symmetrical matrix of 4K x 4K real points following mirror image linear prediction in F1 (64 coefficients) to 128 points.

NOESY spectra were recorded using a phase sensitive experiment with selection gradients during the mixing time. A 300ms mixing time was used for qualitative structural assignment. Data were typically recorded as a matrix of 4096 x 256 complex points and 8 transients per increment. Data were apodized with a $\pi/3$ -shifted squared sine-bell in the F1 dimension truncated at 10%, and with an untruncated $\pi/2$ -shifted squared sine-bell in the F2 dimension. Zero filling was applied in F2 to give a symmetrical matrix of 4K x 4K real points following forward linear prediction in F2 (32 coefficients) to 64 points, and mirror image linear prediction in F1 (64 coefficients) to 128 points.

Carbon chemical shifts were measured from 2D plots of either HSQC spectra for protonated carbons or HMBC spectra for non-protonated carbons. ^1H - ^{13}C HSQC spectra were recorded using a sensitivity improved phase sensitive experiment using an adiabatic shape pulse for ^{13}C inversion, and ^{13}C decoupling during acquisition.⁶ Experimental parameters were optimized for $^1J_{\text{CH}} = 145\text{Hz}$. ^1H -

1. Berger S, Braun S (2004) in *200 and More NMR Experiments*, Wiley-VCH, Weinheim, pp 6-11.

2. a) Claridge TDW (1999) in *High-Resolution NMR Techniques in Organic Chemistry*, Pergamon, Oxford, 1999, 94-97. b) Berger S, Braun S (2004) in *200 and More NMR Experiments*, Wiley-VCH, Weinheim, pp 15-17.

3. a) Hurd R E (1990) Gradient-enhanced spectroscopy. *J Magn Reson* 87(2):422-428. b) Brereton I M, Crozier S, Field J, Doddrell D M (1991) Quadrature detection in F_1 induced by pulsed field gradients. *J Magn Reson* 93(1):54-62. c) Shaw A A, Salaun C, Dauphin J F, Ancian B (1996) Artifact-Free PFG-Enhanced Double-Quantum-Filtered COSY Experiments. *J Magn Reson Ser A* 120(1):110-115.

4. Wagner R, Berger S (1996) Gradient-Selected NOESY—A Fourfold Reduction of the Measurement Time for the NOESY Experiment. *J Magn Reson* 123(1):119-121

5. Cavanagh J, Rance M, (1990) Sensitivity improvement in isotropic mixing (TOCSY) experiments. *J Magn Reson* 88(1):72-85

6. a) Palmer A G III Cavanagh J, Wright P E, Rance M (1991) Sensitivity improvement in proton-detected two-dimensional heteronuclear correlation NMR spectroscopy. *J Magn Reson* 93(1):151-170. b) Kay, L.E.; Keifer, P.; Saarinen, T (1992) Pure absorption gradient enhanced heteronuclear single quantum correlation spectroscopy with improved sensitivity. *J Am Chem Soc* 114(26):10663-10665. c) Schleucher J, et al (1994) A general enhancement scheme in heteronuclear multidimensional NMR employing pulsed field gradients. *J Biomol NMR* 4(2):301-306.

^{13}C HMBC spectra were recorded using a gradient selected experiment with a J -filter element optimized for $^1J_{\text{CH}} = 125\text{-}165\text{Hz}$. Experimental parameters were optimized for long range $^nJ_{\text{CH}} = 8\text{Hz}$.

Solution conformation of compound 39:

The solution conformation of **39** was determined from NMR spectra acquired in 9:1 DMSO- d_6 :H $_2$ O and in 9:1 DMSO- d_6 :D $_2$ O. All spectra were recorded on a Bruker AV-600 spectrometer equipped with an inverse triple resonance probe. Except for variable temperature experiments used for the determination of backbone NH temperature coefficients, all spectra were recorded at 283K. Water suppression was achieved with presaturation for COSY experiments, and with excitation sculpting for 1D- ^1H , TOCSY and NOESY experiments. Sequence specific ^1H assignments were determined by standard methods for unlabeled polypeptides employing TOCSY and NOESY data.⁷ Temperature dependence of backbone H $^{\text{N}}$ chemical shifts was determined from 1D- ^1H experiments and confirmed by COSY experiments.

Distance restraints were obtained from a ^1H - ^1H NOESY experiment using a 150ms mixing time and 2s interscan delay. Data were calibrated to the fixed reference distance Trp H $^{\epsilon 1}$ -H $^{\zeta 2}$ (H18-H20, page 4) of 2.82Å.⁸ Volume integrals were grouped into bins, and classified as strong (<2.5Å), medium (<3.5 Å) or weak (<4.5 Å), based on the relationship of r^{-6} assuming linear buildup and the isolated spin pair approximation. Backbone phi angle restraints were derived from $^3J_{\text{HNHa}}$ coupling constants measured from 1D- ^1H and DQF-COSY experiments conducted in 9:1 DMSO- d_6 :H $_2$ O, and were restrained to $\pm 40^\circ$ of the predicted angle(s) derived the Karplus equation.⁹ Side chain chi-1 torsion restraints were derived from analysis of $^3J_{\text{HaHb}}$ coupling constants measured from 1D- ^1H and E.COSY experiments conducted in 9:1 DMSO- d_6 :D $_2$ O. Stereospecific assignment of β -methylenes was made by analysis of H $^{\text{N}}$ -H $^{\beta}$ NOEs, where possible, and chi-1 angles were restrained to $\pm 60^\circ$ of the predicted angle(s).

Structure calculations were carried out using Macromodel v9.8 (Schrödinger, Inc., San Diego, CA) using the OPLS-2005 force field with implicit GB/SA aqueous solvation and a constant dielectric ($\epsilon = 1.0$). Distance and dihedral restraints were introduced as pseudoenergy terms comprising a flat bottomed harmonic potential of 100kJ/Å 2 , and 1000kJ/mol, respectively. An initial model was generated by a 10,000 step mixed Monte-Carlo long range, low-mode conformational search. Ambiguous NOEs were manually refined based on this initial model. The final structure calculation was carried out in the same manner. Redundant conformers were filtered within a heavy atom RMSD cutoff of 1.0Å, and the top 10 structures selected for the ensemble.

Tabulated NOEs and coupling constants for macrocycle 39 in DMSO- d_6 :H $_2$ O (9:1):

Residue	$^3J_{\text{H}^{\text{N}}\text{H}^{\text{a}}}$ (Hz)	$^3J_{\text{H}^{\text{a}}\text{H}^{\text{b}_i}}$ (Hz)	$^3J_{\text{H}^{\text{a}}\text{H}^{\text{b}}}$ (Hz)
Trp ¹	7.5	5.7 (<i>pro-S</i>)	8.3 (<i>pro-R</i>)
Leu ²	7.0	nd	nd
Gln ³	7.3	5.8 (<i>pro-S</i>)	8.9 (<i>pro-R</i>)
Met ⁴	7.9	4.6 (<i>pro-R</i>)	7.9 (<i>pro-S</i>)
Thr ⁵	7.4	3.8	-
Gly ⁶	na	-	-
Phe ⁷	7.7	4.4 (<i>pro-R</i>)	9.5 (<i>pro-S</i>)
Tyr ⁸	9.1	4.0 (<i>pro-S</i>)	9.6 (<i>pro-R</i>)

7. Cavanagh J, Fairbrother W J, Palmer A G III, Rance M, Skelton NJ (2007) in *Protein NMR Spectroscopy, 2nd Edition: Principles and Practice*. Elsevier Academic Press: San Diego, Ch. 10.

8. Bye E, Mostad A, Romming C (1973) Crystal Structure of DL-Tryptophan Formate. *Acta Chem Scand* 27:471-484.

9. Wang A C, Bax A (1996) Determination of the Backbone Dihedral Angles ϕ in Human Ubiquitin from Reparametrized Empirical Karplus Equations. *J Am Chem Soc* 118(10):2483-2494.

Tabulated NOEs for macrocycle 39

atom A	atom B	volume integral	bin	calc'd structure
18	20	1.00	Ref (2.82Å)	3.0
13	26	1.43	m	4.0
13	23	0.34	m	3.7
13	9	0.22	w	3.4
13	7	0.09	w	4.6
13	15	1.19	m	2.9
13	15'	2.07	m	3.5
13	11	4.69	s	2.3
13	29	0.25	w	3.9
23	14	0.69	m	4.0
23	15'	0.60	m	3.9
23	15	0.66	m	2.4
17	14	0.63	m	3.6
17	15'	0.70	m	2.6
17	15	0.74	m	3.7
17	26	0.20	w	3.8
23	26	0.20	w	3.3
14	26	3.32	s	2.2
15'	26	0.58	m	3.7
15	26	0.69	m	3.7
26	33	1.21	m	4.0
26	30	0.26	w	4.9
26	31	0.35	w	4.5
27	33	3.58	s	2.1
27	30	0.66	w	4.8
27	31	1.92	m	2.3
28	33	1.64	m	2.5
28	40	0.45	m	3.8
28	55	0.27	w	4.0
31	33	0.33	w	3.8
30	33	0.31	w	4.9
33	35	1.87	m	2.5
33	35'	1.40	m	2.9
33	36	1.18	m	4.4
34	40	3.43	s	2.1
34	36	1.75	m	3.2
35	38	0.23	w	2.0
35'	38	0.21	w	3.5
36	38	1.73	m	3.3
36	71	0.63	m	3.5
42	46	0.69	m	3.9
42'	46	0.78	m	3.5
40	46	0.93	m	3.0
40	43	0.66	m	3.7
40	36	0.50	m	3.9
40	42	2.18	m	2.0
40	42'	1.77	m	3.1
41	46	4.56	s	2.9
41	43	0.63	m	2.5
46	52	1.75	m	2.3
46	50	1.15	m	2.6
46	49	1.43	m	2.7
46	43	0.24	w	4.8
47	49	2.14	m	2.6
49	52	0.66	w	4.4
49	55	0.19	w	4.9
50	52	0.53	m	2.6
50	55	0.23	w	2.5
52	55	0.79	m	1.9
52	48	0.87	m	3.7
53'	55	1.74	m	3.3
55	57'	2.02	m	2.5
55	57	2.68	s	2.4
57'	59	1.13	m	3.0
57	59	1.65	m	3.3
56	59	1.03	m	2.3
63	65'	0.99	m	3.7
63	65	2.22	m	2.5
71	63	0.68	m	2.3
64	71	2.52	s	3.2
64	67	2.55	m	3.1
71	65'	0.59	m	4.0
65'	67	2.80	s	2.4
65	67	2.62	s	2.5
63	55	3.13	s	2.6

3	5	1.37	m	3.2
3	9	2.52	s	3.0
2	5	1.19	m	3.7
2	9	2.47	s	2.9
1	5	0.22	w	5.0
1	9	0.29	w	4.1

Total NOE restraints

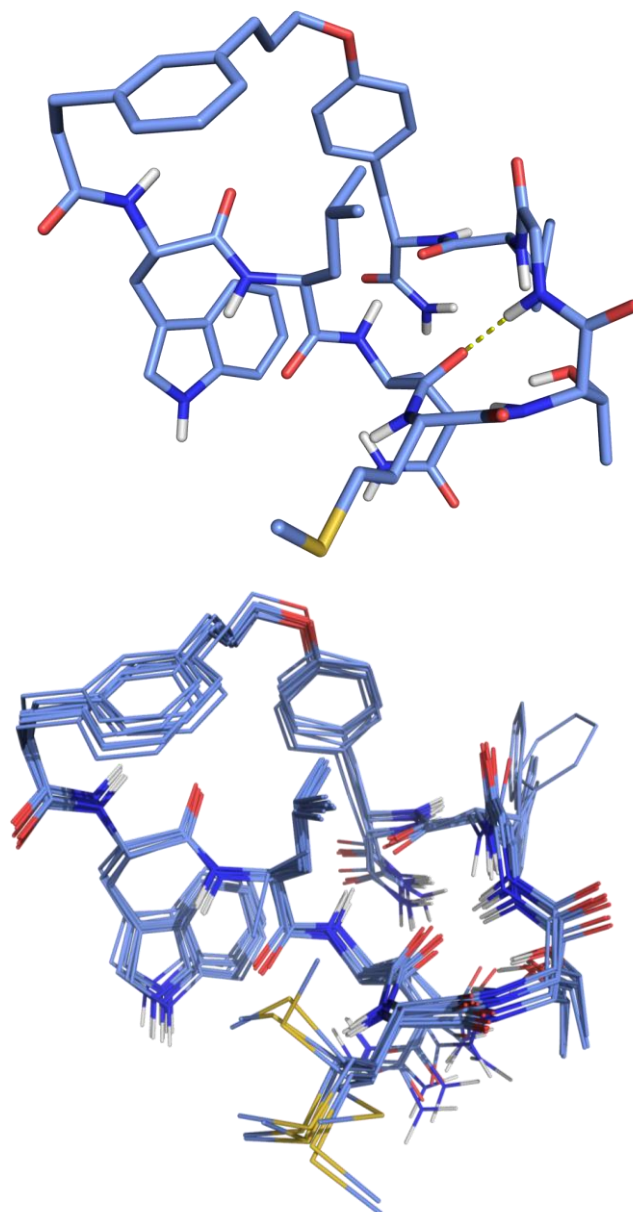
all (80)
 intraresidue (42)
 sequential ($|i - j| = 1$) (31)
 non-sequential, long-range ($|i - j| > 1$) (7)

RMSD (Å) pairwise averaged over ensemble

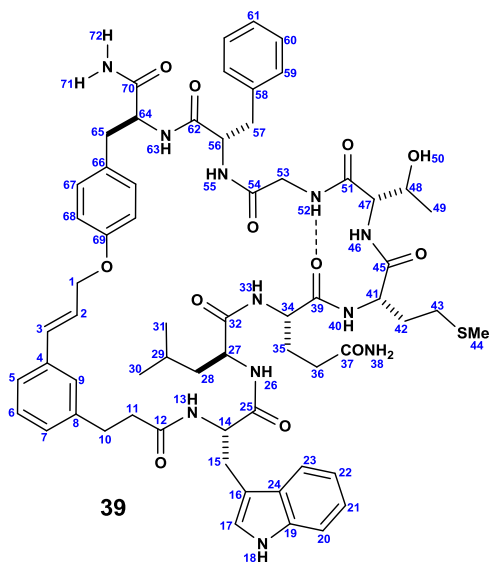
Heavy atoms 0.76
 Core macrocycle 0.36
 All atoms 0.95

Constraint violations

No. of NOEs. > 0.5Å 4
 Sum of violations > 0.5Å (Å) 2.22
 Max. NOE violation (Å) 0.66



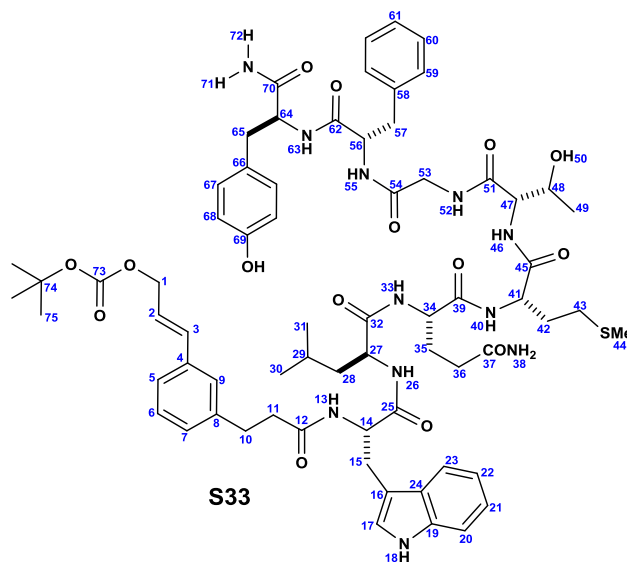
Resonance assignment for WLQMTGFY



reson.	¹³ C	¹ H
1	67.94	4.61
2	124.76	6.40
3	132.25	6.64
4	136.28	-
5	123.67	7.24
6	128.30	7.22
7	127.90	7.03
8	141.64	-
9	126.36	7.22
10	33.42	2.71
11	39.02	2.39
12	172.47	-
13	-	8.11
14	56.70	4.43
15	27.06	2.91, 3.10
16	110.05	-
17	122.96	7.07
18	-	10.74
19	135.91	-
20	111.18	7.31
21	121.03	7.03
22	118.40	6.96
23	118.25	7.53
24	127.29	-
25	172.51	-
26	-	7.83
27	51.52	4.15
28	40.25	1.42
29	21.47	1.42
30	21.47	0.75
31	22.96	0.78
32	172.16	-
33	-	8.01
34	52.62	4.14
35	27.11	1.78,1.91
36	31.27	1.94,2.09
37	174.45	-
38	-	6.74,7.27
39	171.86	-
40	-	7.95
41	51.99	4.39
42	31.20	1.80,1.93
43	29.45	2.35,2.41

9:1 DMSO-*d*₆:H₂O (600 MHz)

reson.	¹³ C	¹ H
44	14.57	1.90
45	171.65	-
46	-	7.70
47	58.59	4.14
48	66.56	3.98
49	19.69	1.01
50	-	5.07
51	171.61	-
52	-	8.01
53	41.93	3.58,3.67
54	170.93	-
55	-	8.08
56	53.98	4.47
57	37.33	2.69,2.98
58	137.75	-
59	129.31	7.17
60	128.56	7.22
61	128.72	7.19
62	168.83	-
63	-	8.00
64	54.35	4.33
65	36.55	2.74,2.94
66	129.95	-
67	129.92	7.14
68	114.38	6.85
69	157.07	-
70	171.24	-
71	-	7.07
72	-	7.25

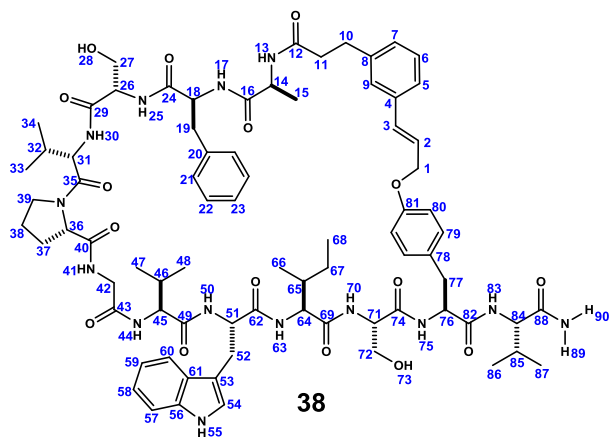


reson.	¹³ C	¹ H
1	-	4.63
2	-	6.28
3	-	6.57
4	-	-
5	-	7.23
6	-	7.23
7	-	6.99
8	-	-
9	-	7.18
10	-	2.65
11	-	2.34
12	-	-
13	-	8.03
14	53.70	4.51
15	-	2.88, 3.09
16	-	-
17	-	7.06
18	-	10.71
19	-	-
20	-	7.31
21	-	7.06
22	-	6.96
23	-	7.56
24	-	-
25	-	-
26	-	8.02
27	51.41	4.25
28	-	1.43
29	-	1.52
30	-	0.79
31	-	0.83
32	-	-
33	-	8.07
34	52.40	4.21
35	-	1.71
36	-	2.12
37	-	-
38	-	6.78, 7.30
39	-	-
40	-	8.10
41	52.15	4.40
42	-	1.81, 1.94
43	-	2.38, 2.44

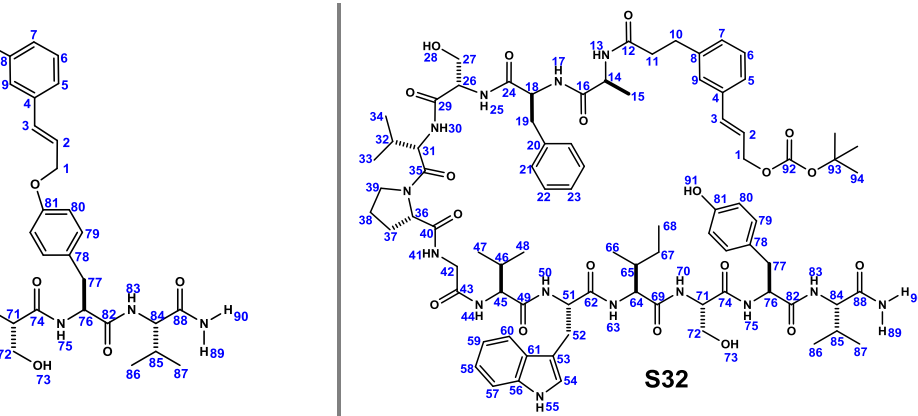
9:1 DMSO-*d*₆:H₂O (600 MHz)

reson.	¹³ C	¹ H
44	-	1.96
45	-	-
46	-	7.70
47	58.62	4.15
48	-	3.97
49	-	1.01
50	-	n/o
51	-	-
52	-	8.05
53	42.17	3.63, 3.68
54	-	-
55	-	8.00
56	54.45	4.41
57	-	2.68, 2.91
58	-	-
59	-	7.13
60	-	7.20
61	-	7.15
62	-	-
63	-	7.97
64	54.60	4.29
65	-	2.70, 2.88
66	-	-
67	-	7.01
68	-	6.63
69	-	-
70	-	-
71	-	7.01
72	-	7.20
73	-	-
74	-	-
75	-	1.40

Resonance assignment for AFSVPGVWISYV



reson.	¹³ C	¹ H
1		4.59
2		6.40
3		6.65
4		-
5		7.23
6		7.24
7		7.08
8		-
9		7.24
10		2.40
11		2.76
12		-
13		8.10
14	49.17	4.05
15		1.02
16		-
17		7.79
18	54.07	4.46
19		2.80, 3.09
20		-
21		7.15
22		7.18
23		7.17
24		-
25		8.00
26	55.23	4.31
27		3.58
28		n/o
29		-
30		7.73
31	55.61	4.33
32		1.96
33		0.81
34		0.86
35		-
36	60.15	4.23
37		1.77, 2.03
38		1.77, 1.90
39		3.53, 3.66
40		-
41		8.29
42	42.30	3.54, 3.77
43		-
44		7.41
45	57.89	4.08
46		1.92
47		0.71
48		0.73



reson.	¹³ C	¹ H
49		-
50		8.10
51	53.78	4.52
52		2.91, 3.07
53		-
54		7.08
55		10.64
56		-
57		7.29
58		7.02
59		6.93
60		7.51
61		-
62		-
63		7.74
64	57.19	4.11
65		1.60
66		0.70
67		0.97, 1.31
68		0.65
69		-
70		7.88
71	55.23	4.28
72		3.52
73		n/o
74		-
75		8.06
76	54.65	4.54
77		2.76, 3.00
78		-
79		7.13
80		6.79
81		-
82		-
83		7.67
84	57.97	4.06
85		1.95
86		0.81
87		0.83
88		-
89		7.08
90		7.33

9:1 DMSO-d₆:H₂O (600 MHz)

reson.	¹³ C	¹ H
1		4.63
2		6.31
3		6.60
4		-
5		7.25
6		7.22
7		7.08
8		-
9		7.26
10		2.37
11		2.74
12		-
13		8.11
14	48.68	4.12
15		1.04
16		-
17		7.96
18	53.85	4.48
19		2.76, 3.03
20		-
21		7.18
22		7.20
23		7.15
24		-
25		8.09
26	55.72	4.32
27		3.55
28		n/o
29		-
30		7.92
31	55.32	4.32
32		1.96
33		0.81
34		0.86
35		-
36	59.92	4.24
37		1.78, 2.02
38		1.78, 1.89
39		3.46, 3.49
40		-
41		8.22
42	42.14	3.63, 3.70
43		-
44		7.61
45	57.74	4.12
46		1.90
47		0.71
48		0.74

reson.	¹³ C	¹ H
49		-
50		8.26
51	53.53	4.53
52		2.91, 3.06
53		-
54		7.08
55		10.72
56		-
57		7.29
58		7.03
59		6.94
60		7.54
61		-
62		-
63		7.89
64	57.23	4.16
65		1.65
66		0.73
67		0.99, 1.33
68		0.73
69		-
70		8.02
71	55.22	4.28
72		3.48, 3.51
73		n/o
74		-
75		8.03
76	54.64	4.42
77		2.71, 2.92
78		-
79		6.98
80		6.58
81		-
82		-
83		7.77
84	57.98	4.03
85		1.92
86		0.79
87		0.81
88		-
89		7.14
90		7.36
91		n/o
92		-
93		-
94		1.39

9:1 DMSO-d₆:H₂O (600 MHz)

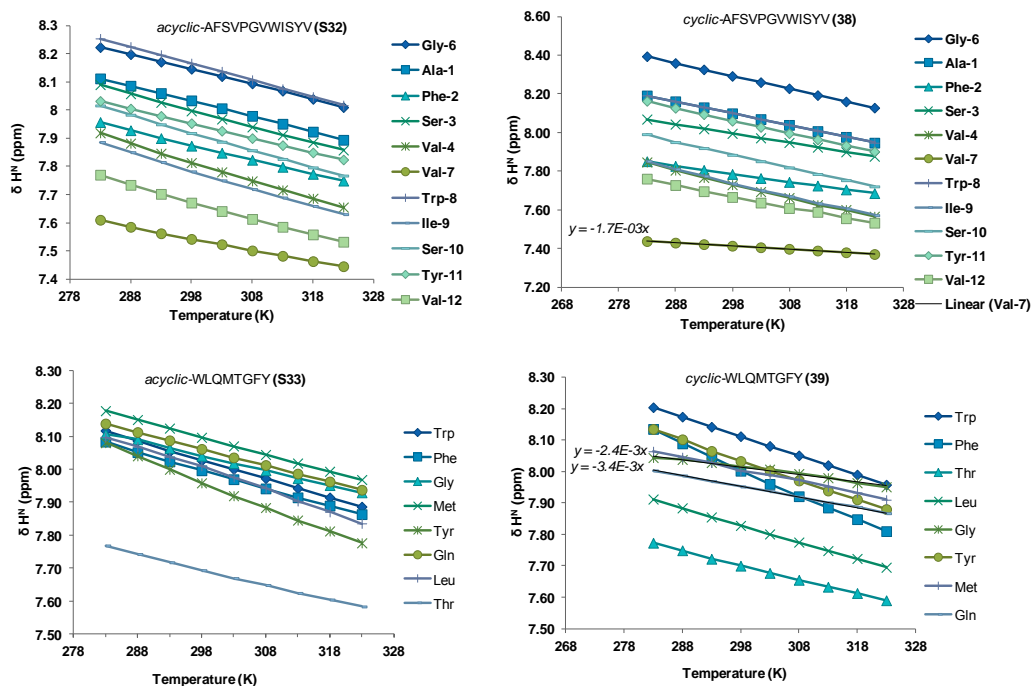
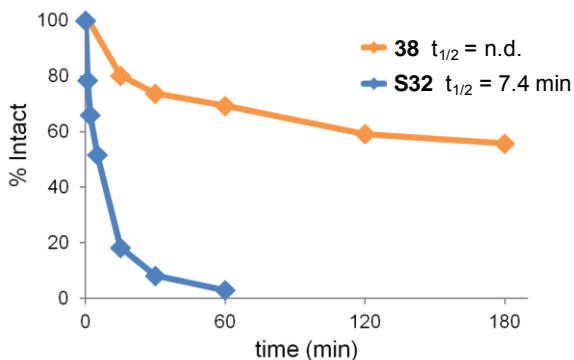


Figure S1. Temperature dependence of backbone $^1\text{H}^{\text{N}}$ chemical shifts for **S32**, **S33**, **38**, and **39**.

Proteolytic degradation assay:

Stock solutions of α -chymotrypsin (bovine type II, 61.75 U/mg) were freshly prepared in 1mM HCl, and diluted into assay buffer (56 mM Tris pH 7.8, 560 μM CaCl_2 , 0.1% v Tween-80) just prior to addition of the substrate. Reactions were conducted in silanized glass vials. The reaction was initiated by addition of DMSO stock solution (50 μM) of the macrocycle **39** or linear precursor **S33** to give a final substrate concentration of 5 μM , 50 $\mu\text{g}/\text{mL}$ α -chymotrypsin, and 10% v DMSO. Control reactions contained BSA instead of α -chymotrypsin. Aliquots were removed in triplicate at 1, 2, 5, 10, 15 and 30 min (acyclic) or 1, 15, 30, 60, 120, and 180 min (cyclic), and diluted 1:1 with *N,N*-DMF containing 1% v TFA, which resulted in a pH < 2. Time course data were obtained by HPLC-MS or HPLC-UV analysis and quantification against external calibration curves. Compound **38** was assayed in the same manner, except that Tween-80 was omitted from the reaction buffer and the initial substrate and enzyme concentrations were 50 μM and 5 $\mu\text{g}/\text{mL}$, respectively. No loss was observed in control reactions. Kinetic constants were determined by least squares fitting to the first order rate law ($\ln[S] = c + A(1 - e^{-kt})$) using the Solver tool in Microsoft Excel. Half lives were calculated as $0.693/k$. α -Chymotrypsin cleavage sites were determined by purification of products from short reaction times, and analysis by HPLC-MS (Agilent 6130) for linear precursors **S32** and **S33** and by infusion ESI-MS/MS (Bruker Solarix) for macrocycles **38** and **39**.



Analytical HPLC conditions for 38:

Column: Agilent Eclipse XBD C18, 4.6x150mm, 5µm

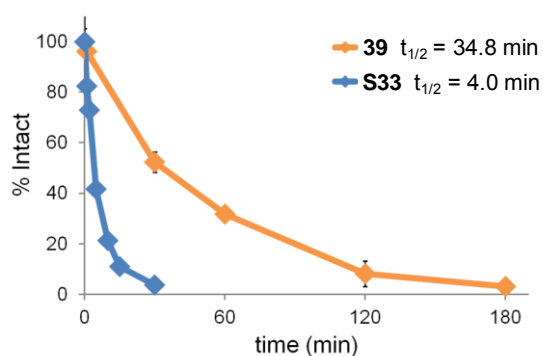
Solvent A: H₂O + 0.1%v TFA

Solvent B: ACN + 0.1%v TFA

Injection Vol.: 40µL

Flow rate: 1.00 ml/min

Time (min)	%B
0.0	30
1.0	30
11.0	100
12.0	30
17.0	30



Analytical HPLC Conditions for 39:

Column: Agilent SB-Aq, 4.6x50mm, 1.8µm

Solvent A: H₂O + 0.1%v TFA

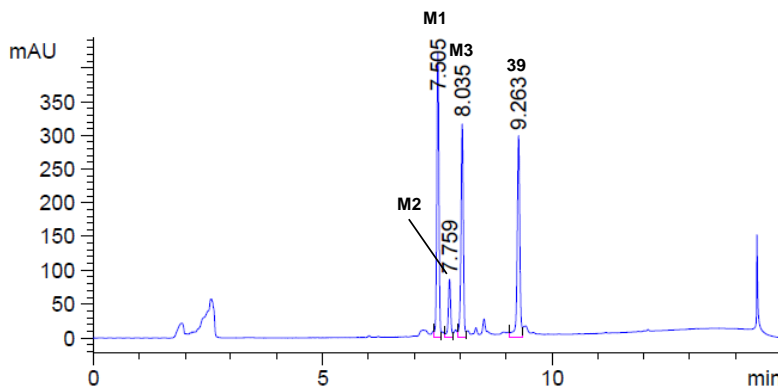
Solvent B: ACN + 0.1%v TFA

Injection Vol.: 40µL

Flow rate: 1.00 ml/min

Time (min)	%B
0.0	30
0.5	30
4.5	100
4.6	30
7.0	30

ESI-MS/MS data for proteolysis of 39



Preparative HPLC Conditions for 39:

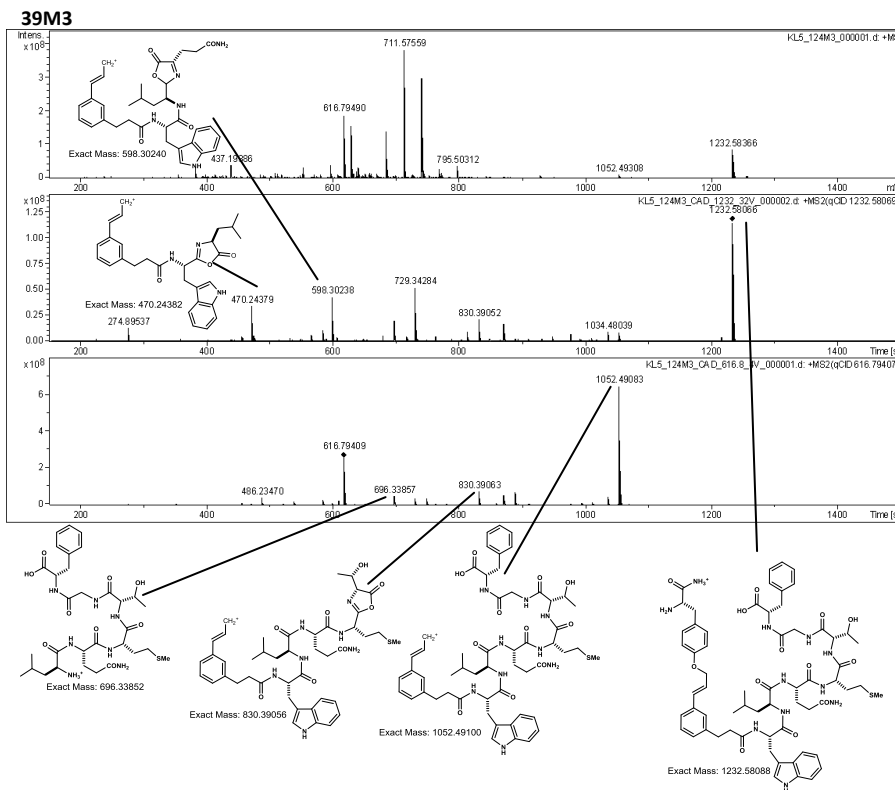
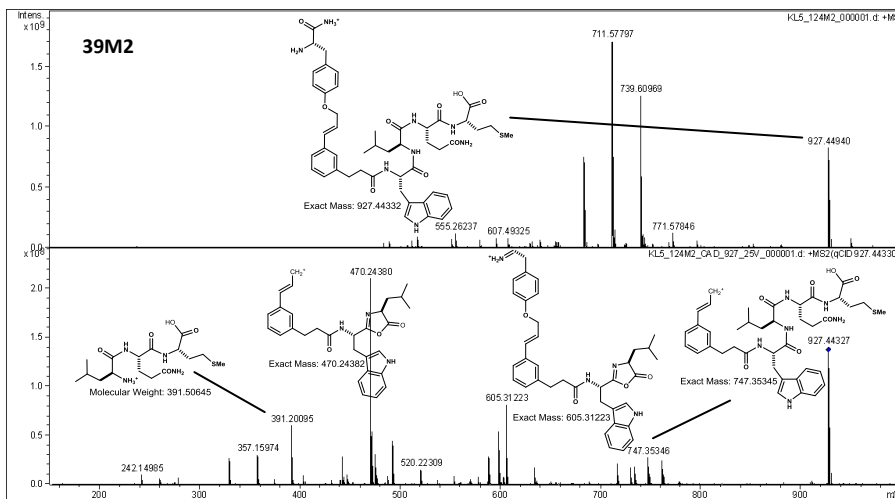
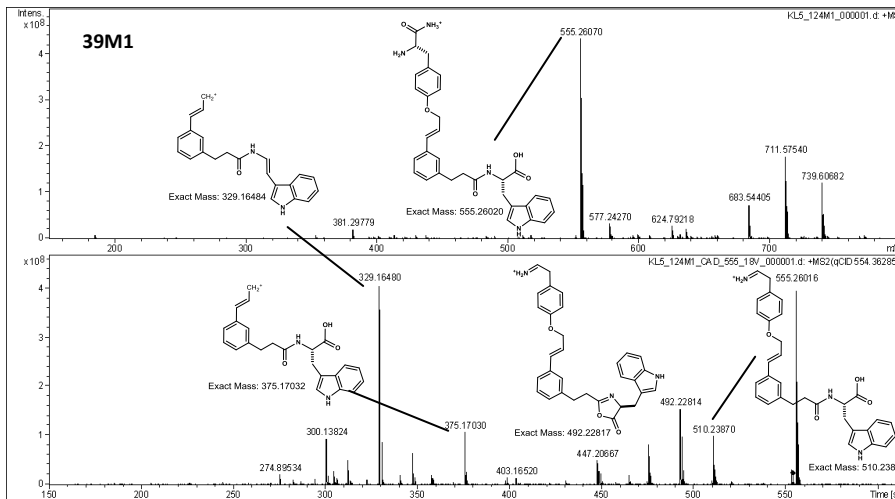
Column: Waters Sunfire, 10x250mm, 5µm

Solvent A: H₂O + 0.1%v TFA

Solvent B: ACN + 0.1%v TFA

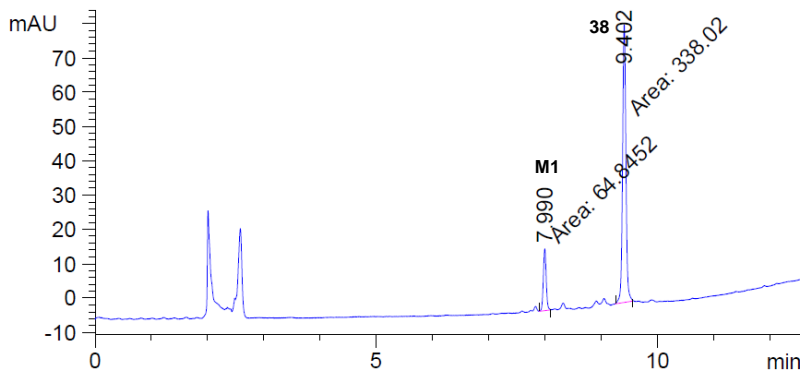
Flow rate: 7.0 ml/min

Time (min)	%B
0.0	20
2.0	20
12.0	100
13.0	20
15.0	20

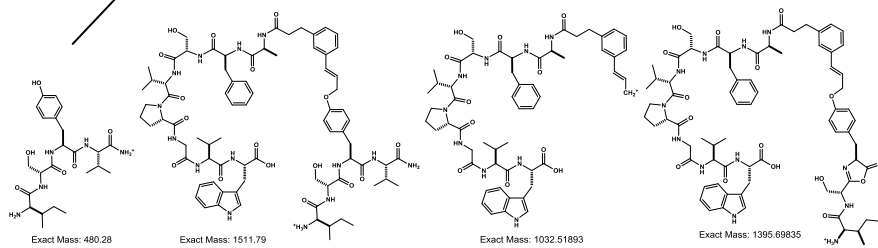
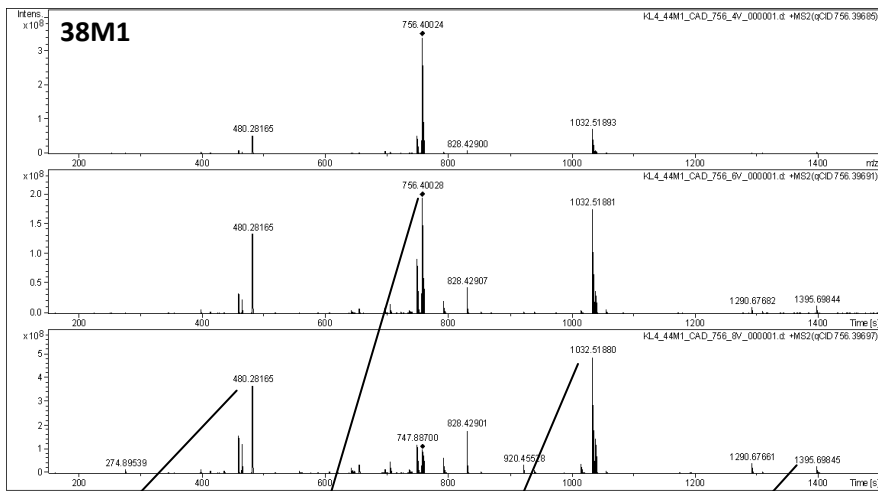


ESI-MS/MS data for proteolysis of 38

Preparative HPLC Conditions for 38:
 Column: Waters Sunfire, 10x250mm, 5µm
 Solvent A: H₂O + 0.1%v TFA
 Solvent B: ACN + 0.1%v TFA
 Flow rate: 7.0 ml/min



Time (min)	%B
0.0	20
2.0	20
12.0	100
13.0	20
15.0	20



Peptide Synthesis:

C-terminal carboxamide peptides were synthesized manually using standard Fmoc solid phase synthesis protocols on Rink Amide MBHA resin (200-400 mesh, 0.70 mmol/g, 1% DVB) on 0.25-0.50 mmolscale using a fritted glass reaction vessel. Fmoc-deprotection was achieved with 20% piperidine in DMF (2 x 30 min). The reaction vessel was washed with DMF (3x) and CH₂Cl₂ (2x). The vessel was then charged with the appropriate Fmoc-amino acid (4 equiv) and TBTU (4 equiv) followed by DMF (10-20 ml) and iPr₂NEt (10 eq). The resin was agitated for 2 hours, drained, and washed with DMF (3X). After all coupling were completed the resin was cleaved with TFA/thioanisole/water/TIPS (90:2.5:5:2.5) for 2 hours. The cleaved resin was removed by filtration and the filtrate was concentrated under vacuum. The peptide was precipitated with ether and isolated by centrifugation. The peptide pellet was repeated washed with Et₂O to ensure complete removal of cleavage reagents. Fmoc-4-(Boc-amino)-L-phenylalanine was used to prepare 4-aminophenylalanine containing peptides.

C-terminal carboxylate peptides were prepared on Wang Resin (0.84 mmol/g). The first amino acid (2.5 equiv) was pre-activated with DIC (2.5 equiv) in DMF (5-10 ml) and then added the pre-swelled resin (1 equiv) and DMAP (0.1 equiv) in DMF (5-10 ml). The resin suspension was agitated for 3 hours. The subsequent Fmoc deprotections, couplings, and resin cleavage were performed as described above.

H-Gly-Trp-Thi-5-Hydroxytryptamine was prepared by attachment of Fmoc-5-hydroxytryptamine to 2-Chlorotritylchloride resin (100-200 mesh, 0.84 mmol/g) via the phenolic oxygen as follows: A solution of Fmoc-5-hydroxytryptamine (398 mg, 1.00 mmol) in dichloromethane (10 ml) was added to a flask containing 2-Chlorotritylchloride resin (840 mg, 1.00 mmol) followed by iPr₂NEt (174 μ l, 1.00 mmol). The mixture was agitated for 10 minutes then an addition aliquot of iPr₂NEt (261 μ l, 1.50 mmol) was added and the mixture was agitated for an addition 2 hours. Methanol (500 μ L) was added and the resin was mixed for an addition 15 minutes, then filtered through a sintered glass funnel. The resin was washed with CH₂Cl₂ (3x), DMF (3x), CH₃OH (3x), and dried under high vacuum. The substitution was estimated by mass. Chain elongation was performed as described above. Cleavage from the resin was achieved with 1:1:8 AcOH:TFE:CH₂Cl₂ for 2 hours.

Synthesis of 1:

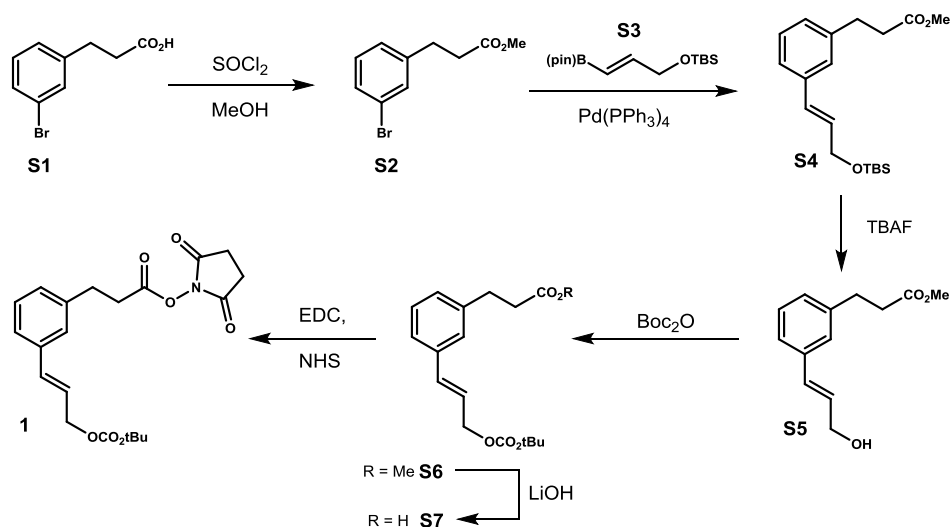


Figure S2. Synthetic route to 1.

methyl 3-(3-bromophenyl)propanoate (S2). To a solution of 3-bromophenylpropanoic acid **S1** (11.52 g, 50.29 mmol) in anhydrous methanol (200 ml) was added dropwise thionyl chloride (7.18 g, 60.35 mmol) over 30 minutes and allowed to stir for 18h at room temperature. Rotary evaporation gave crude ester **S2** as a colorless oil. Purification by column chromatography (SiO₂, 15% EtOAc/hexanes) afforded **S2** (11.80 g, 97%). ¹H NMR (CDCl₃, 500 MHz): δ 7.29-7.35 (m, 2H), 7.08-7.15 (m, 2H), 3.67 (s, 3H), 2.90 (t,

$J = 7.7$ Hz, 2H), 2.62 (t, $J = 7.7$ Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 172.9, 142.9, 131.4, 130.1, 129.4, 127.0, 122.5, 51.7, 35.3, 30.5. MS (ESI) Calculated for $\text{C}_{11}\text{H}_{11}\text{BrO}_2$ $[\text{M}+\text{H}]^+$: 243.0, found 242.6.

(E)-methyl 3-(3-(3-((tert-butyl)dimethylsilyloxy)prop-1-en-1-yl)phenyl)propanoate (S4). To a solution of **S2** (11.80 g, 48.54 mmol) in 4:1 THF/ H_2O (160 ml) was added boronic ester **S3** (17.38g, 58.25 mmol) followed by K_2CO_3 (20.13 g, 145.62 mmol). The resulting suspension was degassed by bubbling Argon through the stirred suspension with a needle for 30 minutes. Following addition of $\text{Pd}(\text{PPh}_3)_4$ (1.68 g, 1.45 mmol) the reaction was heated to 75 °C in an oil bath for 48h or until complete consumption of **S4** determined by HPLC/UV at 220 nm. The reaction was cooled, diluted with EtOAc (250 ml) and washed sequentially water, and brine. The organic layer was dried over Na_2SO_4 , filtered and evaporated to give crude **S3** as an amber viscous oil which was used without further purification. ^1H NMR (CDCl_3 , 500 MHz): δ 7.19-7.25 (m, 3H), 7.04-7.08 (m, 1H), 6.56 (dt, $J = 15.9, 1.7$ Hz, 1H), 6.27 (dt, $J = 15.9, 5.0$ Hz, 1H), 4.34 (dd, $J = 5.0, 1.7$ Hz, 2H), 3.67 (s, 3H), 2.94 (t, $J = 7.9$ Hz, 2H), 2.63 (t, $J = 7.9$ Hz, 2H), 0.94 (s, 9H), 0.11 (s, 6H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 173.4, 140.7, 137.3, 129.32, 129.27, 128.7, 127.3, 126.4, 124.4, 63.9, 51.7, 35.7, 30.9, 26.0, 18.5, -5.1. MS (ESI) Calculated for $\text{C}_{19}\text{H}_{30}\text{O}_3\text{Si}$ $[\text{M}+\text{Na}]^+$: 357.2, found 357.4.

(E)-methyl 3-(3-(3-hydroxyprop-1-en-1-yl)phenyl)propanoate (S5). To a solution of **S4** (16.06 g, 48.0 mmol) in THF (160 ml) at room temperature was added TBAF (1.0M/THF, 64.9 ml, 64.9 mmol). The resulting orange solution was allowed to stir for 2 hours. The reaction mixture was transferred to a separatory funnel, diluted with EtOAc (250 ml) and washed sequentially with sat. NH_4Cl and brine. The organic layer was dried over Na_2SO_4 , filtered, and evaporated in vacuo to give crude **S5** as a viscous amber oil. Purification by column chromatography (SiO_2 , gradient 30-65% EtOAc/hexanes) provides pure cinnamyl alcohol **S5** as a colorless oil (8.95 g, 85%). ^1H NMR (CDCl_3 , 400 MHz): δ 7.16-7.25 (m, 3H), 7.02-7.1 (m, 1H), 6.57 (dt, $J = 16.0, 1.3$ Hz, 1H), 6.33 (dt, 16.0, 5.7 Hz, 1H), 4.29 (dd, $J = 3.7, 3.7$ Hz, 2H), 3.65 (s, 3H), 2.92 (t, $J = 7.9$ Hz, 2H), 2.61 (t, $J = 7.9$ Hz, 2H), 2.29 (br. s, 1H). ^{13}C NMR (CDCl_3 , 100 MHz): δ 173.4, 140.8, 137.0, 130.8, 128.8, 127.6, 126.5, 124.4, 63.5, 51.7, 35.6, 30.8. MS (ESI) Calculated for $\text{C}_{13}\text{H}_{16}\text{O}_3$ $[\text{M}+\text{Na}]^+$: 243.1, found 243.0.

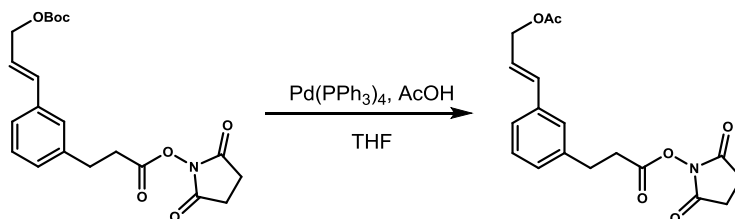
(E)-methyl 3-(3-(3-((tert-butoxycarbonyl)oxy)prop-1-en-1-yl)phenyl)propanoate (S6). To a solution of **S5** (7.5 g, 34.1 mmol) in CH_2Cl_2 (175 ml) at room temperature was added NaOH (15 wt% aqueous, 35 ml) followed by tetrabutylammonium bisulfate (347 mg, 1.02 mmol). Ditertbutyldicarbonate (11.15 g, 51.1 mmol) was subsequently added in one portion and the mixture was allowed to stir overnight at room temperature. The reaction mixture was diluted with CH_2Cl_2 (200 ml) and washed with water and brine. The colorless crude oil obtained (**S6**) was used without further purification. ^1H NMR (CDCl_3 , 500 MHz): δ 7.20-7.25 (m, 3H), 7.06-7.12 (m, 1H), 6.63 (br. d, $J = 15.9$ Hz, 1H), 6.27 (dt, $J = 15.9, 6.4$ Hz, 1H), 4.70 (dd, $J = 6.4, 1.2$ Hz, 2H), 3.66 (s, 3H), 2.93 (t, $J = 7.9$ Hz, 2H), 2.62 (t, $J = 7.9$ Hz, 2H), 1.49 (s, 9H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 173.3, 153.4, 140.9, 136.4, 134.3, 128.8, 128.1, 126.7, 124.7, 123.0, 82.2, 67.5, 51.7, 35.6, 30.8, 27.8. MS (ESI) Calculated for $\text{C}_{18}\text{H}_{24}\text{O}_5$ $[\text{M}+\text{Na}]^+$: 343.2, found 343.2.

(E)-3-(3-(3-((tert-butoxycarbonyl)oxy)prop-1-en-1-yl)phenyl)propanoic acid (S7). Crude methyl ester **S6** (10.92 g, 34.1 mmol) was dissolved in THF (170 ml) and aqueous LiOH (1.0 M, 52.0 ml) was added. The reaction was stirred for 4 hours at room temperature. The reaction was then diluted with EtOAc (300 ml) and 1.0 M HCl was added until the aqueous layer has a pH < 2. The organic layer was separated and washed with water and brine, dried over Na_2SO_4 , filtered and the solvent was removed by rotary evaporation to give **S7** (8.4 g, 80% over 2 steps) as an oil which was >95% pure by HPLC/UV. ^1H NMR (CDCl_3 , 500 MHz): δ 7.21-7.27 (m, 3H), 7.08-7.13 (m, 1H), 6.64 (d, $J = 15.9$ Hz, 1H), 6.29 (dt, $J = 15.8, 6.4$ Hz, 1H), 4.71 (br. d, $J = 6.3$ Hz, 2H), 2.95 (t, $J = 7.9$ Hz, 2H), 2.7 (t, $J = 7.8$ Hz, 1H), 1.5 (s, 9H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 178.0, 153.4, 140.5, 136.5, 134.3, 128.9, 128.1, 126.7, 124.8, 123.1, 82.3, 67.4, 35.3, 30.5, 27.8. MS (ESI-Neg) Calculated for $\text{C}_{17}\text{H}_{22}\text{O}_5$ $[\text{M}-\text{H}]^-$: 305.1, found 305.2.

(E)-2,5-dioxopyrrolidin-1-yl 3-(3-(3-((tert-butoxycarbonyl)oxy)prop-1-en-1-yl)phenyl)propanoate (1).

To a solution of **S7** (5.9 g, 19.3 mmol) in CH_2Cl_2 (60 ml, 0.35 M) at room temperature was added N-hydroxysuccinimide (2.66g, 23.11 mmol) followed by EDC-HCl (4.06 g, 21.18 mmol). The reaction was stirred for 3 hours then transferred to a separatory funnel and washed sequentially with 1N HCl, H_2O and brine. The organic layer was dried over Na_2SO_4 , filtered and concentrated to give an amber oil. Purification by column chromatography (SiO_2 , 35% EtOAc/hexane) afforded succinimidyl ester **1** as a white solid (6.09 g, 15.1 mmol, 78 %). Analytically pure crystals may be obtained by slow evaporation from THF/hexanes (2:1). ^1H NMR (CDCl_3 , 500 MHz): δ

7.24-7.28 (m, 3H), 7.11-7.15 (m, 1H), 6.65 (br. d, J = 15.9 Hz, 1H), 6.3 (dt, J = 15.9, 6.4 Hz, 1H), 4.72 (dd, J = 6.4, 1.3 Hz, 2H), 3.05 (t, J = 7.8 Hz, 2H), 2.92 (t, J = 7.8 Hz, 2H), 2.84 (br. s, 4H), 1.5 (s, 9H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 169.0, 167.8, 153.4, 139.4, 136.7, 134.1, 129.0, 128.0, 126.7, 125.1, 123.3, 82.2, 67.4, 32.6, 30.4, 27.8, 25.6. IR (neat) ν = 2947, 1820, 1781, 1732, 1370, 1269, 1252, 1211, 1160, 1068, 972, 930, 793 cm^{-1} . MS (ESI) Calculated for $\text{C}_{21}\text{H}_{25}\text{NO}_7$ $[\text{M}+\text{Na}]^+$: 426.2, found 426.2.



(E)-2,5-dioxopyrrolidin-1-yl 3-(3-(3-acetoxyprop-1-en-1-yl)phenyl)propanoate (S8). A solution of 1 (558 mg, 1.38mmol, 1 equiv.) and AcOH (1.97 mL, 34.5mmol, 25 equiv.) in THF (20 ml) was sparged with argon for 15 minutes. The septa was removed briefly to allow the addition of Pd(PPh₃)₄ (40 mg, 0.035mmol, 2.5 mol%). The reaction was stirred for 4 hours then diluted with EtOAc and transferred to a separatory funnel. The organic layer was washed with saturated aq. NaHCO₃, H₂O, and brine, dried over Na₂SO₄ and evaporated to give a yellow solid. Purification by column chromatography (SiO₂, gradient 20-60% EtOAc/Hexane) afforded the title compound (443 mg, 1.28mmol, 93 %) as a off-white solid. NMR (CDCl_3 , 500 MHz): δ 7.22-7.25 (m, 3H), 7.08-7.12 (m, 1H), 6.61 (dt, J = 16.0, 1.1 Hz, 1H), 6.27 (dt, J = 16.0, 6.4 Hz, 1H), 4.7 (dd, J = 6.4, 1.3 Hz, 2H), 3.02 (t, J = 7.8 Hz, 2H), 2.89 (t, J = 7.7 Hz, 2H), 2.79 (br. s, 4H), 2.08 (s, 3H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 170.8, 169.2, 167.9, 139.5, 136.6, 133.8, 129.0, 128.0, 126.6, 125.0, 123.6, 65.0, 32.5, 30.3, 25.6, 21.0. MS (ESI) Calculated for $\text{C}_{18}\text{H}_{19}\text{NO}_6$ $[\text{M}+\text{Na}]^+$: 368.1, found 368.1

Coupling of 1 to acyclic peptides:

General Procedure A. An oven-dried, screw-capped scintillation vial was charged with appropriate peptide (0.2 mmol) and N-hydroxysuccinimidyl ester 1 (0.20 mmol) followed by addition of anhydrous DMF (2 ml, 0.10 M) and *i*Pr₂NEt (0.8 mmol, 4 equiv.). The reaction was allowed to stir at room temperature until complete conversion as monitored by LC/MS. The solvent is removed under reduced pressure and purified as described below. Compounds purified by preparative HPLC were treated with silica bound tetraalkylammonium carbonate (Si-CO₃, Silicycle, 0.59 mmol/g, 2 equiv.) for 30 minutes in DMF, and re-concentrated to scavenge residual TFA prior to cyclization.

Palladium-catalyzed macrocyclization:

General Procedure B. An oven-dried vial was charged with acyclic peptide (0.05mmol) and sealed with a septa. The vial was flushed with Argon followed by addition of argon-sparged anhydrous DMF (10 ml, 5 mM). After complete dissolution of the peptide, Pd(PPh₃)₄ (0.0025mmol, 5 mol %) in 1:1 THF:DMF (0.5 ml) was added and the reaction was allowed to stir at room temperature for two hours or until complete conversion of starting material as monitored by LC/MS. The solvent is removed under reduced pressure. The resulting residue is reconstituted in DMSO and purified by preparative HPLC as indicated below.

General Procedure C. A solution of catalyst was prepared as follows: An oven-dried, serum-topped vial was placed in a glove bag and charged with [PdCl(C₃H₅)₂]₂ (14 mg, 0.038mmol) and xantphos (55 mg, 0.095mmol). The vial is sealed, removed from the glove bag, and degassed THF (7.0 ml) was added, followed by degassed DMF (7.0 ml). The resulting yellow solution was stirred under argon for 30 minutes.

To a solution of acyclic peptide (0.05 mmol) in degassed DMF (10 ml, 5 mM) was added catalyst solution (735 μL , 0.04 mol% [PdCl(C₃H₅)₂]₂, 0.10 mol% xantphos). The reaction was allowed to stir at room temperature for two hours or until complete conversion of starting material as monitored by LC/MS. The solvent is removed under reduced pressure. The resulting residue is reconstituted in DMSO and purified by preparative HPLC as indicated below.

General Procedure D. As described in general procedure B with the addition of Cs₂CO₃. An oven-dried vial was charged with acyclic peptide (0.05 mmol) and Cs₂CO₃ (0.10 mmol, 2 equiv) and sealed with a septa. The vial was flushed with Argon followed by addition of

argon-sparged anhydrous DMF or DMSO (10 ml, 5 mM). After complete dissolution of the peptide, Pd(PPh₃)₄ (0.0025 mmol, 5 mol %) in 1:1 THF:DMF (0.5 ml) was added and the reaction was allowed to stir at room temperature for two hours or until complete conversion of starting material as monitored by LC/MS. The solvent is removed under reduced pressure. The resulting residue is reconstituted in DMSO and purified by preparative HPLC as indicated below.

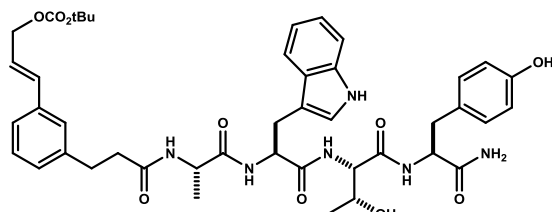
Summary of acylation of macrocyclization efficiency.

Peptide Sequence	Yield % (acylation)	Cyclization Procedure	Yield % (cyclization)	Peptide Sequence	Yield % (acylation)	Cyclization Procedure	Yield % (cyclization)
S M Y	71	B	80	A V P H	78	C	77
I W Y	65	B	72	G ^{Thi} W 5HT	57	B	75
A V Y	67	B	78	A F S V P G V W I S Y V	72	B	66
A W T Y	72	B	78	T A W I P Y H N V	64	C	69
V M F Y	59	B	73	W L Q M T G F Y	64	B	71
W I Q Y	70	B	81	B-Ala-P(4-Ar)-H	78	C	81
L A R Y	66	B	84	G T H Y	68	C	73
I M S Y W	77	B	73	A R H F	63	C	76
A F T I Y	67	B	85	A I H F	72	C	71
G S F N Y	80	B	74	V Q Y H	56	C	75
S F F(4-NH₂)	62	B	72	V Q Y H	-	C ^a	68
A L E Y	68	B	67	H-V O M Y	62	D ^a	64
A L E Y	-	D	76	H-VO M Y	-	B	77
FLHyp- OH	57	B	71	N W T F(4-NH₂)	61	B	77
G V W- OH	61	B	74	Orn T Y	97	D ^a	80
AVP H-OH	74	C	69				

^aDMSO Solvent.

Data for acyclic peptides:

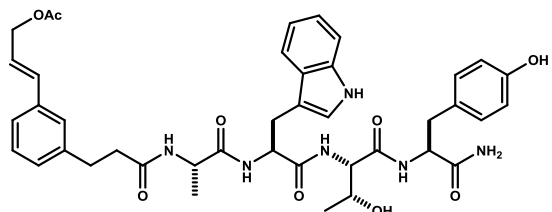
Acyclic-Ala-Trp-Thr-Tyr (2):



Following general procedure A, the corresponding compound was prepared from H-AWTY-NH₂ (•TFA, 163 mg, 0.250 mmol), diisopropylethylamine (174 μL, 0.999 mmol) and reagent 1 (101 mg, 0.250 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (149 mg, 0.180 mmol, 72%). ¹H NMR (DMSO-d₆, 600 MHz): δ 10.76

(s, 1H), 9.13 (br s, 1H), 8.05 (d, J = 7.9 Hz, 1H), 7.99 (d, J = 7.3 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.67 (d, J = 7.7 Hz, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.22-7.31 (m, 4H), 7.19 (dd, J = 7.6, 7.6 Hz, 1H), 7.10 (app s, 2H), 7.60 (d, J = 7.4 Hz, 1H), 6.96-7.02 (m, 3H), 6.89 (dd, J = 7.4, 7.4 Hz, 1H), 6.57-6.63 (m, 3H), 6.30 (dt, 15.9, 6.3 Hz, 1H), 4.63 (d, J = 5.8 Hz, 2H), 4.52 (ddd, J = 8.2, 8.2, 4.8 Hz, 1H), 4.33 (ddd, J = 8.2, 8.2, 5.2 Hz, 1H), 4.24 (dq, J = 7.1, 7.1 Hz, 1H), 4.16 (dd, J = 7.9, 4.1 Hz, 1H), 3.89-3.96 (m, 1H), 3.12 (dd, J = 15.0, 4.2 Hz, 1H), 2.95 (dd, J = 14.8, 9.0 Hz, 1H), 2.90 (dd, J = 14.0, 4.9 Hz, 1H), 2.65-2.78 (m, 3H), 2.28-2.41 (m, 2H), 1.39 (s, 9H), 1.08 (d, J = 6.8 Hz, 3H), 0.90 (d, J = 6.4 Hz, 3H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.2, 172.8, 171.7, 171.6, 169.6, 156.1, 153.1, 142.1, 136.3, 136.2, 133.8, 130.3, 128.9, 128.4, 128.1, 127.7, 126.7, 124.6, 123.9, 123.6, 121.1, 118.7, 118.5, 115.2, 111.5, 110.3, 81.8, 67.2, 66.9, 58.3, 54.6, 53.8, 48.4, 36.9, 36.9, 31.2, 27.7, 19.3, 18.4. MS (ESI) Calculated for C₄₄H₅₄N₆O₁₀ [M-OCO₂tBu]⁺: 709.3, found 709.0.

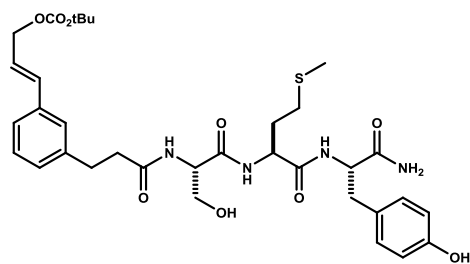
Acyclic-Ala-Trp-Thr-Tyr (3):



Following general procedure A, the corresponding compound was prepared from H-AWTY-NH₂ (•TFA, 195 mg, 0.299 mmol), diisopropylethylamine (208 μL, 1.19 mmol) and reagent **S8** (103 mg, 0.299 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100%

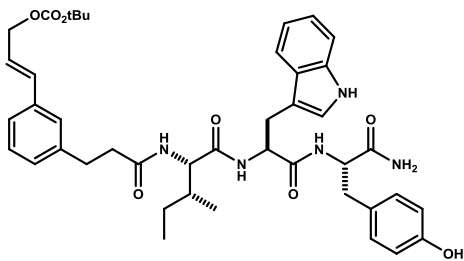
CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (177 mg, 0.230 mmol, 77%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.77 (d, J = 1.9 Hz, 1H), 9.13 (br. s, J = Hz, 1H), 8.05 (d, J = 7.5 Hz, 1H), 7.99 (d, J = 7.3 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.54 (d, J = 7.9 Hz, 1H), 7.18-7.32 (m, 5H), 7.09-7.13 (m, 2H), 7.07 (br. d, J = 7.3 Hz, 1H), 6.98-7.04 (m, 3H), 6.9 (dd, J = 7.4 Hz, 1H), 6.58-6.64 (m, 3H), 6.31 (dy, J = 15.9, 6.1 Hz, 1H), 4.65 (br. d, J = 6.1 Hz, 2H), 4.53 (ddd, J = 8.3, 8.3, 4.6 Hz, 1H), 4.34 (ddd, J = 8.2, 8.2, 5.3 Hz, 1H), 4.25 (dq, J = 7.2, 7.2 Hz, 1H), 4.18 (dd, J = 8.2, 4.2 Hz, 1H), 3.90-3.97 (m, 1H), 3.13 (dd, J = 15.1, 4.4 Hz, 1H), 2.97 (dd, J = 15.2, 8.7 Hz, 1H), 2.91 (dd, J = 14.1, 5.1 Hz, 1H), 2.66-2.79 (m, 3H), 2.28-2.43 (m, 2H), 2.03 (s, 3H), 1.1 (d, J = 7.1 Hz, 3H), 0.92 (d, J = 6.6 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.4, 172.9, 171.9, 171.7, 170.6, 169.8, 156.2, 142.2, 136.5, 136.4, 133.6, 130.5, 129.1, 128.4, 128.3, 127.8, 126.8, 124.7, 124.1, 124.0, 121.3, 118.9, 118.7, 115.4, 111.7, 110.4, 67.0, 64.8, 58.4, 54.7, 53.9, 48.6, 37.1, 37.0, 31.4, 27.5, 21.2, 19.5, 18.6. MS (ESI) Calculated for C₄₁H₄₈N₆O₉ [M+H]⁺: 769.3, found 769.2.

Acyclic-Ser-Met-Tyr (S9):



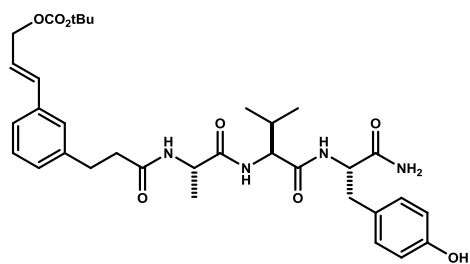
Following general procedure A, the corresponding compound was prepared from H-SMY-NH₂ (•TFA, 20 mg, 0.039 mmol), diisopropylethylamine (27 μL, 0.156 mmol) and reagent **1** (16 mg, 0.039 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (19 mg, 0.028mmol, 71%). ¹H NMR (DMSO-d₆, 400 MHz): δ 9.14 (br s, 1H), 8.28 (d, J = 6.8 Hz, 1H), 8.04 (d, J = 7.9 Hz, 1H), 7.77 (d, J = 8.4 Hz, 1H), 7.18-7.29 (m, 3H), 7.12 (br s, 1H), 7.08 (d, J = 7.08 Hz, 1H), 7.06 (br s, 1H), 6.95 (d, J = 8.4 Hz, 2H), 6.57-6.63 (m, 3H), 6.31 (dt, J = 16, 6.3 Hz, 1H), 4.64 (dd, 6.3, 1.0 Hz, 2H), 4.34 (ddd, J = 7.0, 7.0, 6.8 Hz, 1H), 4.23 (ddd, J = 9.8, 8.7, 4.6 Hz, 1H), 4.89 (ddd, J = 8.6, 7.1, 4.7 Hz, 1H), 3.57 (dd, J = 10.3, 6.1 Hz, 1H), 3.47 (dd, J = 10.3, 6.9 Hz, 1H), 2.91 (dd, J = 14.0, 4.5 Hz, 1H), 4.77 (t, J = 8 Hz, 2H), 2.54-5.62 (m, 1H), 2.41-2.48 (m, 4H), 2.30-2.37 (m, 1H), 2.23-2.29 (m, 1H), 1.95 (s, 3H), 1.39 (s, 9H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.4, 172.0, 171.5, 170.9, 156.1, 153.1, 142.1, 136.2, 133.8, 130.2, 128.9, 128.4, 128.2, 126.7, 124.6, 123.6, 115.2, 81.8, 67.2, 62.1, 55.0, 54.6, 53.0, 40.8, 36.9, 36.8, 31.3, 31.2, 29.6, 27.7, 14.8. MS (ESI) Calculated for C₃₄H₄₆N₄O₉S [M-OCO₂tBu]⁺: 569.2, found 568.9.

Acyclic-Ile-Trp-Tyr (S10):



Following general procedure A, the corresponding compound was prepared from H-IWY-NH₂ (•TFA, 203 mg, 0.342 mmol), diisopropylethylamine (238 μL, 1.37 mmol) and reagent **1** (138 mg, 0.342 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (171 mg, 0.222mmol, 65%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.78 (d, J = 1.4 Hz, 1H), 9.12 (s, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.82 (d, J = 8.6 Hz, 1H), 7.74 (d, J = 8.1 Hz, 1H), 7.51 (d, J = 8 Hz, 1H), 7.26-7.30 (m, 2H), 7.17-7.25 (m, 3H), 7.06-7.10 (m, 2H), 7.00-7.05 (m, 1H), 6.92-6.97 (m, 3H), 6.57-6.64 (m, 3H), 6.31 (dt, J = 15.9, 6.3 Hz, 1H), 4.65 (d, J = 6.1 Hz, 2H), 4.48 (ddd, J = 8.3, 8.3, 4.9 Hz, 1H), 4.62 (ddd, J = 7.8, 7.8, 5.9 Hz, 1H), 4.11 (ddd, J = 8.2, 8.2 Hz, 1H), 3.02 (ddd, J = 14.9, 4.5 Hz, 1H), 2.89 (ddd, J = 14.9, 8.9 Hz, 1H), 2.67-2.84 (m, 4H), 2.36 (ddd, J = 14.5, 8.6, 5.9 Hz, 1H), 1.52-1.62 (m, 1H), 1.41 (s, 9H), 1.32-1.39 (m, 1H), 1.15-1.26 (m, 1H), 0.83-0.95 (m, 1H), 0.69 (t, J = 7.3 Hz, 3H), 0.64 (d, J = 6.9 Hz, 3H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 172.9, 171.7, 171.5, 171.2, 161.8, 156.1, 153.1, 142.0, 136.3, 136.1, 133.8, 130.4, 128.9, 128.4, 128.0, 127.6, 126.7, 124.5, 123.7, 123.5, 121.1, 118.6, 118.5, 115.2, 111.5, 110.3, 81.8, 67.2, 57.2, 54.3, 53.8, 40.8, 37.1, 36.8, 36.6, 31.3, 27.7, 24.5, 24.3, 15.5, 11.2. MS (ESI) Calculated for C₄₃H₅₃N₅O₈ [M-OCO₂tBu]⁺: 650.3, found 649.9.

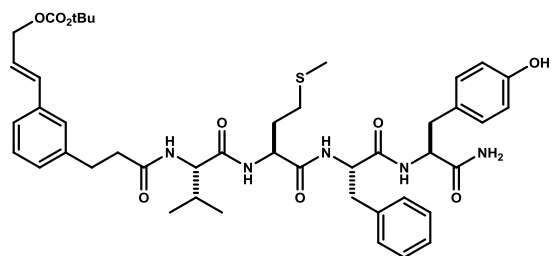
Acyclic-Ala-Val-Tyr (S11):



Following general procedure A, the corresponding compound was prepared from H-AVY-NH₂ (+TFA, 18 mg, 0.039 mmol), diisopropylethylamine (27 μ L, 0.155 mmol) and reagent 1 (16 mg, 0.039 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (17 mg, 0.026mmol, 17%). ¹H NMR (DMSO-d₆, 400 MHz): δ 9.11 (br s, 1H), 8.04 (d, J = 7.3 Hz, 1H), 7.92 (s, 1H), 7.45 (d, J = 8.6 Hz, 1H), 7.70 (d, J = 8.9 Hz), 7.26 (br s, 1H), 7.22-7.26 (m, 2H), 7.20 (app t, J = 7.5 Hz, 1H),

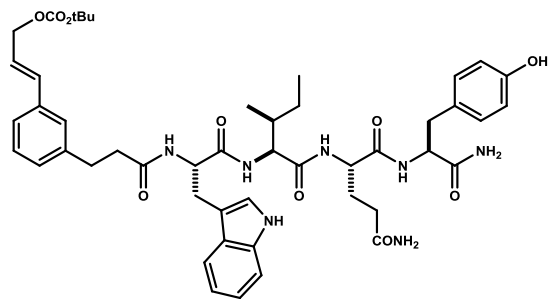
7.08 (d, J = 7.4 Hz, 1H), 7.00 (br s, 1H), 6.95 (d, J = 8.3 Hz, 1H), 6.56-6.63 (m, 2H), 6.31 (dt, J = 15.8, 6.3 Hz, 1H), 4.64 (d, J = 6.06 Hz, 2H), 4.26-4.36 (m, 2H), 4.03 (dd, J = 8.4, 6.7 Hz, 1H), 2.83 (dd, J = 13.9, 5.2 Hz, 1H), 2.76 (t, J = 7.7 Hz, 2H), 2.66 (dd, J = 14.0, 8.9 Hz), 2.34-2.44 (m, 1H), 1.88 (dddd, J = 13.3, 6.6, 6.6, 6.6 Hz, 1H), 1.39 (s, 9H), 1.10 (d, J = 7.2 Hz, 3H), 0.71 (d, J = 6.4 Hz, 6H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.2, 172.7, 171.6, 170.7, 156.1, 153.1, 142.0, 136.2, 133.8, 130.3, 128.9, 128.4, 128.1, 126.7, 124.6, 123.6, 115.1, 81.8, 67.2, 58.2, 54.1, 48.4, 40.8, 37.1, 36.9, 31.2, 30.7, 27.7, 19.4, 18.3, 18.2. MS (ESI) Calculated for C₃₄H₄₆N₄O₈ [M-OC(=O)C(CH₃)₃]⁺: 521.3, found 521.0.

Acyclic-Val-Met-Phe-Tyr (S12):



Following general procedure A, the corresponding compound was prepared from H-VMFY-NH₂ (+TFA, 149 mg, 0.222 mmol), diisopropylethylamine (155 μ L, 0.887 mmol) and reagent 1 (89 mg, 0.222 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (111 mg, 0.131mmol, 59%). ¹H NMR (DMSO-d₆, 600 MHz): δ 9.13 (s, 1H), 8.00 (d, J = 7.7 Hz, 1H), 7.92 (d, J = 7.9 Hz, 1H), 7.83-7.90 (m, 2H), 7.27 (s, 1H), 7.10-7.25 (m, 9H), 7.08 (d, J = 7.2 Hz, 1H), 7.03 (s, 1H), 6.97 (d, J = 8.1 Hz, 2H), 6.57-6.65 (m, 2H), 6.30 (dt, J = 16.0, 6.0 Hz, 1H), 4.63 (d, J = 6.1 Hz, 2H), 4.45 (ddd, J = 8.2, 8.2, 4.8 Hz, 1H), 4.22-4.35 (m, 2H), 4.07 (dd, J = 7.5, 7.5 Hz, 1H), 2.9 (dd, J = 14.0, 4.2 Hz, 1H), 2.64-2.88 (m, 6H), 2.48-2.56 (m, 1H), 2.26-2.44 (m, 3H), 1.95 (d, 3H), 1.74-1.90 (m, 2H), 1.64-1.73 (m, 1H), 1.39 (s, 9H), 0.69 (d, J = 6.6 Hz, 6H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.0, 172.0, 171.5, 171.1, 170.7, 156.1, 153.1, 142.0, 137.9, 136.2, 133.8, 130.4, 129.4, 128.9, 128.4, 128.3, 128.0, 126.7, 126.5, 124.6, 123.6, 115.2, 81.8, 67.2, 58.2, 54.4, 54.1, 52.2, 37.7, 37.2, 36.8, 32.0, 31.3, 30.5. MS (ESI) Calculated for C₄₅H₅₉N₅O₉S [M+Na]⁺: 868.4, found 868.9.

Acyclic-Trp-Ile-Gln-Tyr (S13):

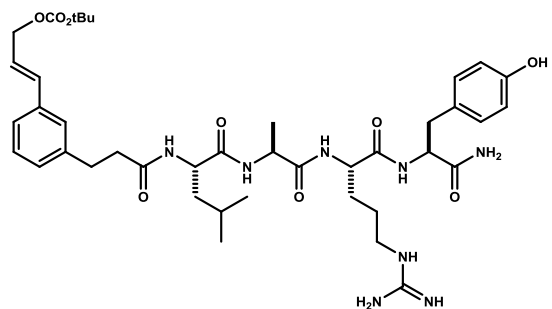


Following general procedure A, the corresponding compound was prepared from H-WIQY-NH₂ (+TFA, 77 mg, 0.107 mmol), diisopropylethylamine (74 μ L, 0.427 mmol) and reagent 1 (43 mg, 0.107 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (67 mg, 0.075mmol, 70%). ¹H NMR (DMSO-d₆, 400 MHz): δ 10.73 (s, 1H), 9.12 (br s, 1H), 8.02-8.06 (m, 2H), 7.90 (d, J = 8.1 Hz, 1H), 7.79 (d, J = 7.9 Hz, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.30 (br s, 1H), 7.18-7.25 (m, 3H), 7.14 (dd, J =

7.7, 7.7 Hz, 1H), 6.99-7.06 (m, 3H), 6.91-6.99 (m, 4H), 6.478 (br s, 1H), 6.58 (d, J = 7.9 Hz, 2H), 6.56 (d, J = 15.3 Hz, 1H), 6.29 (dt, J = 16.0, 6.2 Hz, 1H), 4.62 (d, J = 6.2 Hz, 2H), 4.58 (ddd, J = 9.3, 9.3, 4.7 Hz, 1H), 4.30 (ddd, J = 7.6, 7.6, 7.6 Hz, 1H), 4.20 (ddd, J = 7.7, 7.7, 7.7 Hz, 1H), 4.14 (dd, J = 7.7, 7.7 Hz, 1H), 3.07 (dd, J = 14.7, 4.1 Hz, 1H), 2.87 (dd, J = 14.6, 9.5 Hz, 1H), 2.82 (dd, J = 14.0, 5.3 Hz, 1H), 2.60-2.66 (m, 2H), 2.32 (dd, J = 7.7, 7.7 Hz, 1H), 2.03-2.08 (m, 1H), 1.81 (dddd, J = 13.8, 6.4, 6.4, 6.4 Hz, 1H), 1.64-1.74 (m, 2H), 1.39 (s, 9H), 0.97-1.07 (m, 1H), 0.76 (t, J = 7.3 Hz, 3H), 0.75 (d, J = 6.8 Hz, 3H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 174.3, 173.1, 172.0, 171.7, 171.2, 171.0, 156.1, 153.1, 142.0, 136.3, 136.1, 133.8, 130.3, 128.9, 128.2, 128.0, 127.7, 126.7, 124.5, 123.9, 123.6,

121.1, 118.9, 118.5, 115.2, 111.5, 110.5, 81.8, 67.2, 57.4, 54.4, 53.6, 52.7, 40.4, 37.2. MS (ESI) Calculated for $C_{48}H_{61}N_7O_{10}$ $[M-OCO_2tBu]^+$: 778.4, found 777.9.

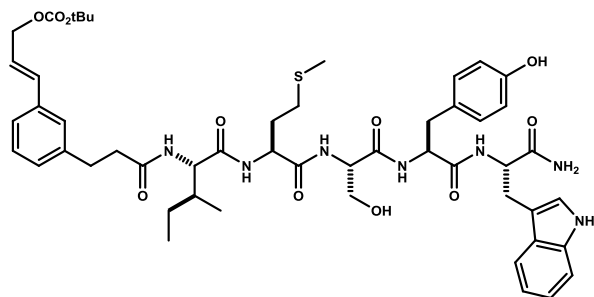
Acyclic-Ile-Ala-Arg-Tyr (S14):



Following general procedure A, the corresponding compound was prepared from H-LARY-NH₂ (\cdot 3TFA, 88 mg, 0.102 mmol), diisopropylethylamine (71 μ L, 0.408 mmol) and reagent 1 (41 mg, 0.102 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 20-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (54 mg, 0.067 mmol, 67%). ¹H NMR (DMSO-d₆, 600 MHz): δ 8.06 (d, J = 6.8 Hz, 1H), 7.94-7.99 (m, 2H), 7.88 (d, J = 7.7 Hz, 1H), 7.73 (d, J = 7.9 Hz, 1H), 7.55 (dd, J = 5.5, 5.5 Hz, 1H), 7.31 (s, 1H), 7.22-7.27 (m, 2H), 7.19 (dd, J =

7.7, 7.7 Hz, 1H), 7.07 (d, J = 7.4 Hz, 1H), 7.04 (s, 1H), 6.95 (d, J = 8.5 Hz, 2H), 6.56-6.62 (m, 3H), 6.30 (dt, J = 16.2, 6.5 Hz, 1H), 4.63 (d, J = 6.2 Hz, 2H), 4.29 (ddd, J = 8.1, 8.1, 5.4 Hz, 1H), 4.24 (dq, J = 7.8, 7.8 Hz, 1H), 4.12-4.20 (m, 2H), 2.99-3.05 (m, 2H), 2.80-2.87 (m, 2H), 2.72-2.79 (m, 2H), 2.65-2.69 (m, 1H), 2.55 (d, J = 4.7 Hz, 1H), 2.43-2.49 (m, 2H), 2.35-2.42 (m, 1H), 1.59 (dddd, J = 14.3, 6.7, 6.7, 6.7 Hz, 1H), 1.43-1.51 (m, 1H), 1.39 (s, 9H), 1.31-1.37 (m, 2H), 1.15 (d, J = 7.3 Hz, 3H), 0.78 (d, J = 6.4 Hz, 3H), 0.72 (d, J = 6.6 Hz, 3H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.1, 172.6, 172.6, 171.9, 171.1, 161.9, 159.0 (TFA, q, J = 34.5 Hz), 157.1, 156.1, 153.1, 141.9, 136.2, 133.8, 130.4, 128.9, 128.4, 128.0, 126.7, 124.5, 123.6, 116.6 (TFA, q, J = 295 Hz) 115.2, 81.8, 67.2, 54.3, 52.6, 51.2, 48.7, 40.9, 40.7, 37.1, 36.8, 31.2, 29.3, 27.7, 25.1, 24.3, 23.4, 21.7, 18.0. MS (ESI) Calculated for $C_{41}H_{60}N_8O_9$ $[M+H]^+$: 809.4, found 809.0.

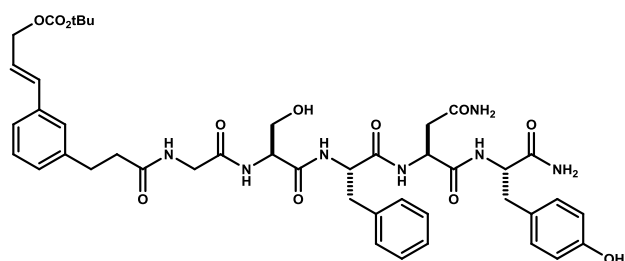
Acyclic-Ile-Met-Ser-Tyr-Trp (S15):



Following general procedure A, the corresponding compound was prepared from H-IMSYW-NH₂ (\cdot TFA, 211 mg, 0.292 mmol), diisopropylethylamine (204 μ L, 1.17 mmol) and reagent 1 (118 mg, 0.292 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (202 mg, 0.225 mmol, 77%). ¹H NMR (DMSO-d₆, 400 MHz): δ 10.78 (s, 1H), 8.02-8.10 (m, 2H), 7.95 (d, J = 8.2 Hz, 1H), 7.91 (d, J = 6.8 Hz, 1H), 7.78 (d, J = 7.3 Hz, 1H), 7.54 (d, J = 7.7 Hz, 1H),

7.29 (d, J = 7.9 Hz, 1H), 7.7 (br s, 1H), 7.21-7.25 (m, 1H), 7.19 (dd, J = 7.6, 7.6 Hz, 1H), 7.14 (br s, 1H), 7.06-7.11 (m, 3H), 7.02 (dd, J = 7.4, 7.4 Hz, 1H), 6.95 (dd, J = 7.4, 7.4 Hz, 1H), 6.88 (d, J = 8.3 Hz, 2H), 6.60 (d, J = 15.9 Hz, 1H), 6.54 (d, J = 8.3 Hz, 2H), 6.30 (dt, J = 16.2, 6.4 Hz, 1H), 4.63 (d, J = 5.5 Hz, 2H), 4.63 (ddd, J = 8.3, 8.3, 5.6 Hz, 1H), 4.23-4.35 (m, 3H), 7.09 (dd, J = 8.2, 8.2 Hz), 3.55 (dd, J = 10.5, 5.9 Hz, 1H), 3.45 (dd, J = 10.4, 6.6 Hz, 1H), 3.12 (dd, J = 14.4, 5.0 Hz, 1H), 2.88 (dd, J = 15.1, 8.9 Hz), 2.71-2.82 (m, 3H), 2.60 (dd, J = 14.3, 9.1 Hz, 1H), 2.30-2.43 (m, 4H), 1.82-1.90 (1H), 1.70-1.79 (m, 1H), 1.57-1.65 (m, 1H), 1.39 (s, 9H), 1.23-1.32 (m, 1H), 0.90-1.0 (m, 1H), 0.67-0.74 (m, 6H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.6, 171.8, 171.7, 171.3, 170.9, 170.5, 156.1, 153.1, 141.9, 136.4, 136.1, 133.8, 130.3, 128.9, 128.4, 127.9, 127.6, 126.7, 124.5, 123.8, 123.6, 121.2, 118.7, 118.6, 115.2, 111.6, 110.5, 81.8, 67.2, 62.0, 57.2, 55.2, 55.1. MS (ESI) Calculated for $C_{51}H_{67}N_7O_{11}S$ $[M-OCO_2tBu]^+$: 868.4, found 867.9.

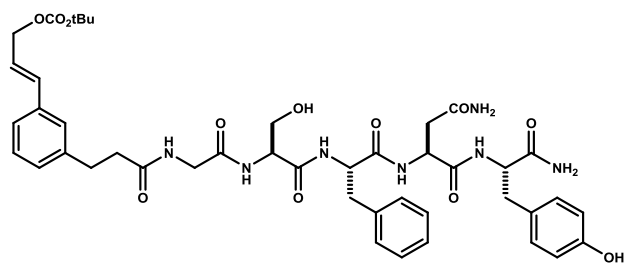
Acyclic-Ala-Phe-Thr-Ile-Tyr (S16):



Following general procedure A, the corresponding compound was prepared from H-AFTIY-NH₂ (\cdot TFA, 31 mg, 0.043 mmol), diisopropylethylamine (30 μ L, 0.171 mmol) and reagent 1 (17 mg, 0.043 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1%

TFA. The fractions collected were combined and lyophilized (26 mg, 0.029mmol, 67%). ¹H NMR (DMSO-d₆, 400 MHz): δ 8.00 (d, J = 8.28 Hz, 1H), 7.99 (d, J = 7.92 Hz, 1H), 7.87 (d, J = 8.1 Hz, 1H), 7.75 (d, J = 7.9 Hz, 1H), 7.69 (d, J = 8.1 Hz, 1H), 7.16-7.26 (m, 7H), 7.11-7.15 (m, 1H), 7.10 (br s, 1H), 7.07 (d, J = 7.9 Hz, 1H), 7.03 (br s, 1H), 6.95 (d, J = 8.9 Hz, 2H), 6.56-6.62 (m, 3H), 6.30 (dt, J = 15.8, 6.2 Hz, 1H), 4.63 (dd, J = 6.0, 0.9 Hz, 2H), 4.53 (ddd, J = 8.8, 8.8, 4.3 Hz, 1H), 4.25-4.35 (m, 2H), 4.21 (dq, J = 7.2, 7.2 Hz), 4.10 (dd, J = 7.7, 6.4 Hz, 1H), 3.95-4.02 (m, 1H), 3.03 (dd, J = 14.2, 4.1 Hz, 1H), 2.85-2.90 (m, 1H), 2.80 (dd, J = 14.1, 9.9 Hz, 1H), 2.70-2.76 (m, 2H), 2.61 (dd, J = 13.9, 9.5 Hz, 1H), 2.29-2.42 (m, 2H), 1.62-1.71 (m, 1H), 1.39 (s, 9H), 1.11-1.21 (m, 1H), 1.06 (d, J = 7.0 Hz, 3H), 0.99 (d, J = 6.6 Hz, 3H), 0.67-0.74 (m, 6H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.2, 172.6, 171.6, 171.3, 170.7, 170.3, 156.1, 153.1, 142.0, 138.1, 136.2, 133.8, 130.2, 129.6, 129.0, 128.4, 128.3, 128.2, 126.7, 126.5, 124.6, 123.6, 115.2, 81.8, 67.2, 67.0, 58.0, 57.7, 54.5, 54.1, 48.4, 40.8, 37.3, 36.9, 36.88, 36.80, 36.1, 31.2, 27.7, 24.1, 19.5, 18.4, 15.6, 11.6. MS (ESI) Calculated for C₄₈H₆₄N₆O₁₁ [M+H]⁺: 901.5, found 901.0.

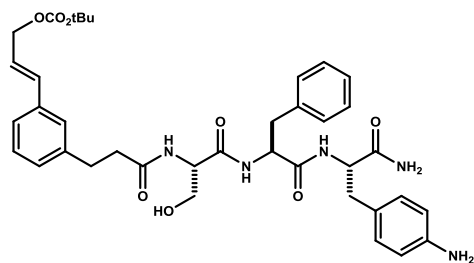
Acyclic-Gly-Ser-Phe-Asn-Tyr (S17):



Following general procedure A, the corresponding compound was prepared from H-GSFNY-NH₂ (•TFA, 120 mg, 0.172 mmol), diisopropylethylamine (119 μL, 0.686 mmol) and reagent 1 (69 mg, 0.172 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (120 mg, 0.137mmol, 80%). ¹H NMR (DMSO-d₆, 600 MHz): δ 8.14 (d, J = 6.6 Hz,

1H), 8.08-8.12 (m, 1H), 8.02 (d, J = 7.1 Hz, 1H), 7.89-7.94 (m, 2H), 7.87 (d, J = 7.2 Hz, 1H), 7.40 (app. s, 1H) 7.34 (app s, 1H) 7.06-7.30 (m, 10H), 7.93-7.99 (m, 3H), 7.56-7.63 (m, 3H), 6.31 (dt, J = 15.7, 6.6 Hz, 1H), 4.64 (d, J = 4.9 Hz, 2H), 4.41-4.50 (m, 2H), 4.18-4.26 (2H), 4.67-4.73 (m, 2H), 3.43-3.50 (m, 2H), 2.97 (d, J = 12.7 Hz, 1H), 2.92 (d, J = 13.2 Hz, 1H), 2.72-2.80 (m, 3H), 2.39-2.57 (m, 3H), 2.35 (dd, J = 15.1, 5.1 Hz, 1H), 1.39 (s, 9H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 173.2, 172.2, 172.0, 171.2, 170.7, 170.3, 169.5, 153.1, 142.1, 138.0, 136.2, 133.8, 130.3, 129.5, 129.0, 128.3, 126.8, 124.5, 123.6, 115.2, 81.8, 67.2, 61.9, 55.4, 54.8, 54.4, 50.2, 42.4, 37.3. MS (ESI) Calculated for C₄₄H₅₅N₇O₁₂ [M+H]⁺: 874.4, found 874.0

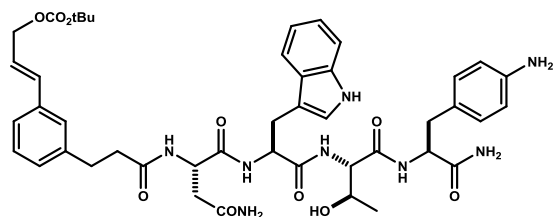
Acyclic-Ser-Phe-Phe(4-NH₂) (S18):



Following general procedure A, the corresponding compound was prepared from H-SFF(4-NH₂)-NH₂ (•2TFA, 170 mg, 0.265 mmol), diisopropylethylamine (185 μL, 1.06 mmol) and reagent 1 (107 mg, 0.265 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 30-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (115 mg, 0.164mmol, 62%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.08 (d, J = 7.7 Hz, 1H), 8.05 (d, J = 8.1 Hz, 1H), 7.97 (d, J = 7.7 Hz, 1H), 7.22-7.28 (m, 3H), 7.16-7.28 (m, 4H), 7.12-7.15 (m, 4H), 7.1 (d,

J = 8.5 Hz, 2H), 7.07 (d, J = 7.6 Hz, 1H), 6.6 (d, J = 15.8 Hz, 1H), 6.31 (dt, J = 16.1, 6.2 Hz, 1H), 6.64 (dd, J = 6.1, 1.0 Hz, 2H), 4.32-4.38 (m, 2H), 4.28 (ddd, J = 6.8, 6.8, 6.8 Hz, 1H), 3.41-3.50 (m, 2H), 3 (dd, J = 13.7, 4.8 Hz, 1H), 2.92 (dd, J = 14.1, 4.5 Hz, 1H), 2.68-2.78 (m, 4H), 2.34-2.45 (m, 2H), 1.39 (s, 9H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 173.0, 172.6, 172.1, 171.5, 170.4, 157.2, 153.3, 142.1, 136.5, 136.3, 133.9, 130.7, 129.1, 128.4, 127.8, 126.9, 124.7, 124.1, 123.8, 121.3, 119.0, 118.6, 118.3, 115.9, 111.7, 110.6, 82.0, 67.4, 67.0, 58.5, 54.5, 54.0, 52.7, 40.9, 40.6. MS (ESI) Calculated for C₃₈H₄₇N₅O₈ [M+H]⁺: 702.3, found 702.3.

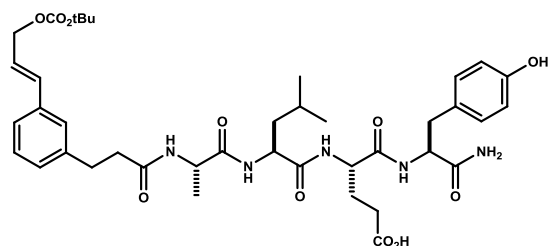
Acyclic-Asn-Trp-Thr-Phe(4-NH₂) (S19):



Following general procedure A, the corresponding compound was prepared from H-NWTF(4-NH₂)-NH₂ (•2TFA, 162 mg, 0.200mmol), diisopropylethylamine (140μL, 0.801mmol) and reagent 1 (81 mg, 0.200mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient

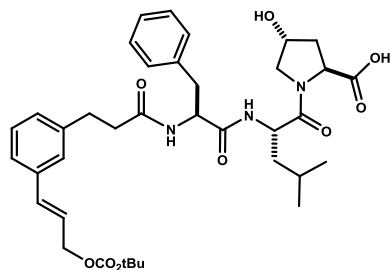
of 30-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (106 mg, 0.122mmol, 61%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.8 (d, J = 1.9 Hz, 1H), 8.09 (d, J = 7.8 Hz, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.9 (d, J = 8.3 Hz, 1H), 7.77 (d, J = 8.3 Hz, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.4 (br. s, J = Hz, 1H), 7.33 (br. s, J = Hz, 1H), 7.24-7.31 (m, 5H), 7.21 (dd, J = 7.8, 7.8 Hz, 1H), 7.11-7.19 (m, 4H), 7.08 (br. d, J = 7.3 Hz, 1H), 7.01 (dd, J = 7.1, 7.1 Hz, 1H), 6.97 (br. s, J = Hz, 1H), 6.91 (dd, J = 7.4, 7.4 Hz, 1H), 6.62 (d, J = 16 Hz, 1H), 6.32 (dt, J = 15.9, 6.2 Hz, 1H), 4.65 (dd, J = 6.3, 1.1 Hz, 2H), 4.56 (dq, J = 7.3, 7.3 Hz, 1H), 4.5 (ddd, J = 5.1, 5.1, 4.5 Hz, 1H), 4.41 (ddd, J = 8.5, 8.5, 5.2 Hz, 1H), 4.12 (dd, J = 8.0, 4.50 Hz, 1H), 3.92 (dddd, J = 12.5, 6.2, 6.2, 6.2 Hz, 1H), 3.15 (dd, J = 14.7, 4.0 Hz, 1H), 3.07 (dd, J = 13.9, 4.9 Hz, 1H), 2.98 (dd, J = 15.0, 8.7 Hz, 1H), 2.82 (dd, J = 13.8, 8.7 Hz, 1H), 2.66-2.76 (m, 2H), 2.44-2.54 (m, 1H), 2.27-2.39 (m, 3H), 1.41 (s, 9H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 173.1, 172.3, 172.0, 171.9, 171.7, 170.0, 153.3, 142.2, 137.5, 136.5, 136.3, 133.9, 131.8, 130.9, 129.1, 128.5, 127.8, 126.9, 124.7, 124.1, 123.8, 122.5, 121.3, 118.8, 118.7, 111.7, 110.3, 82.0, 67.4, 67.1, 59.1, 54.4, 54.1, 50.1, 37.5, 37.2, 31.4, 27.85, 27.78, 27.5, 19.7. MS (ESI) Calculated for C₄₅H₅₆N₈O₁₀ [M+H]⁺: 869.4, found 869.3.

Acyclic-Ala-Leu-Glu-Tyr (15):



Following general procedure A, the corresponding compound was prepared from H-ALEY-NH₂ (•TFA, 183 mg, 0.301 mmol), diisopropylethylamine (210 μL, 1.205 mmol) and reagent 1 (122 mg, 0.301 mmol). The product was isolated by flash chromatography (SiO₂, gradient 0-10% CH₃OH/CHCl₃). The fractions collected were combined and concentrated under reduced pressure (160 mg, 0.205mmol, 68%). ¹H NMR (DMSO-d₆, 400 MHz): δ 8.04 (d, J = 6.8 Hz, 1H), 7.96 (d, J = 7.2 Hz, 1H), 7.82 (d, J = 7.1 Hz, 1H), 7.72 (d, J = 8.1 Hz, 1H), 7.17-7.30 (m, 4H), 7.08 (d, J = 7.0 Hz, 1H), 7.02 (s, 1H), 6.96 (d, J = 7.7 Hz, 2H), 6.56-6.64 (m, 3H), 6.31 (dt, J = 15.8, 6.2 Hz, 1H), 4.64 (d, J = 5.3 Hz, 2H), 4.12-4.31 (m, 4H), 2.72-2.83 (m, 3H), 2.62-2.68 (m, 1H), 2.49-2.54 (m, 1H), 2.44-2.48 (m, 2H), 2.36-2.43 (m, 2H), 2.11-2.20 (m, 2H), 1.78-1.88 (m, 1H), 1.64-1.74 (m, 1H), 1.51-1.59 (m, 1H), 1.35-1.46 (m, 10H), 1.12 (d, J = 7.1 Hz, 3H), 0.84 (d, J = 6.4 Hz, 3H), 0.79 (d, J = 6.2 Hz, 3H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 174.3, 173.0, 172.8, 172.3, 171.7, 170.9, 156.1, 153.1, 142.1, 136.2, 133.8, 130.3, 128.9, 128.4, 128.0, 126.7, 124.5, 123.6, 115.2, 81.8, 67.2, 54.4, 52.3, 51.5, 48.5, 37.0, 36.9, 34.7, 31.2, 30.3, 27.7, 27.6, 24.5, 23.3, 21.9, 18.3. MS (ESI) Calculated for C₄₀H₅₅N₅O₁₁ [M-OCO₂tBu]⁺: 666.4, found 664.0.

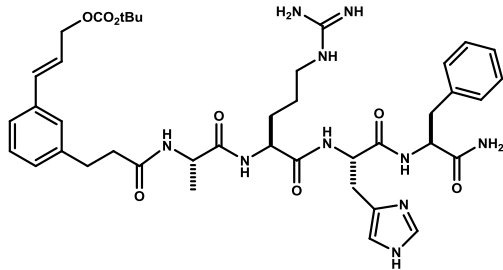
Acyclic-Phe-Leu-Hyp (S21):



Following general procedure A, the corresponding compound was prepared from H-FLHyp-OH (•TFA, 215 mg, 0.425 mmol), diisopropylethylamine (296 μL, 1.70 mmol) and reagent 1 (172 mg, 0.425 mmol). The product was isolated by flash chromatography (SiO₂, gradient 0-10% CH₃OH/CHCl₃). The fractions collected were combined and concentrated under reduced pressure (165 mg, 0.242mmol, 57%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.10 (d, J = 8.3 Hz, 1H), 8.01 (d, J = 8.6 Hz, 1H), 7.12-7.26 (m, 8H), 7.00 (d, J = 7.4 Hz, 1H), 6.60 (d, J = 15.9 Hz, 1H), 6.31 (dt, J = 15.9, 6.3 Hz, 1H), 4.65 (dd, J = 6.1, 1.1 Hz, 2H), 4.50-4.55 (m, 2H), 4.31-4.37 (m, 1H), 3.59 (dd, J = 10.2, 4.6 Hz, 1H), 3.50-3.56 (m, 1H), 2.96 (dd, J = 13.9, 4.0 Hz, 1H), 2.60-2.72 (m, 3H), 2.29-2.35 (m, 2H), 2.07 (ddd, J = 11.9, 8.0, 2.5 Hz, 1H), 1.89 (ddd, J = 12.8, 8.0, 4.8 Hz, 1H), 1.62 (dddd, J = 13.4, 13.4, 6.9, 6.9 Hz, 1H), 1.41 (s, 9H), 0.86-0.89 (m, 6H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 171.7, 171.5, 170.8, 153.3, 142.2, 138.4, 136.3, 133.9, 129.6, 129.1, 128.4, 126.9, 126.6, 124.6, 123.7, 82.0, 69.4, 67.4, 58.2, 55.1, 54.0, 49.0, 40.7, 38.1, 37.6, 37.2, 31.4, 27.8, 24.4, 23.6, 22.1. MS (ESI) Calculated for C₃₇H₄₉N₃O₉ [M-OCO₂tBu]⁺: 562.3, found 562.4.

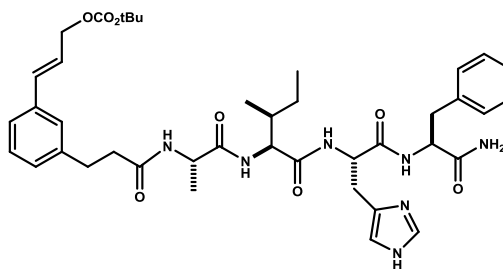
133.6, 133.4, 129.9, 128.6, 128.0, 126.3, 124.2, 123.2, 116.7, 81.5, 66.9, 59.8, 55.8, 51.3, 48.5, 47.7, 36.5, 30.8, 30.1, 28.9, 27.3, 26.3, 24.7, 18.8. MS (ESI) Calculated for $C_{36}H_{51}N_7O_8[M+H]^+$: 710.4, found 710.4.

Acyclic-Ala-Arg-His-Phe-NH₂ (S25):



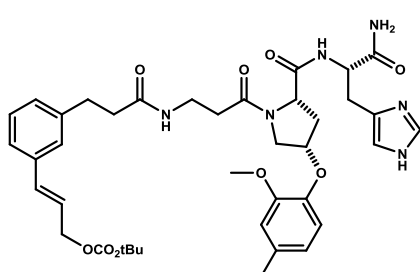
Following general procedure A, the corresponding compound was prepared from H-ARHF-NH₂ (\cdot 4TFA, 54 mg, 0.055 mmol), diisopropylethylamine (38 μ L, 0.219 mmol) and reagent 1 (22 mg, 0.055 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 10-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (28 mg, 0.035mmol, 63%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.94 (d, J = 1.2 Hz, 1H), 8.03-8.11 (m, 4H), 7.63 (dd, J = 5.6 Hz, 1H), 7.59 (br. s, 1H), 7.20-7.29 (m, 9H), 7.15-7.19 (m, 1H), 7.09 (br. d, J = 7.4 Hz, 1H), 6.62 (br. d, J = 15.9 Hz, 1H), 6.32 (dt, J = 16.0, 6.3 Hz, 1H), 4.65 (dd, J = 6.1, 1.1 Hz, 2H), 4.53 (ddd, J = 7.8, 7.8, 5.9 Hz, 1H), 4.41 (ddd, J = 8.6, 8.2, 4.9 Hz, 1H), 4.23 (dq, J = 7.0, 7.0 Hz, 1H), 4.17 (ddd, J = 7.8, 7.8, 5.6 Hz, 1H), 2.98-3.07 (m, 4H), 2.97 (dd, J = 15.7, 8.0 Hz, 1H), 2.74-2.85 (m, 3H), 2.35-2.46 (m, 2H), 1.57-1.60 (m, 1H), 1.43-1.53 (m, 2H), 1.41 (s, 9H), 1.12 (d, J = 7.2 Hz, 3H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 173.4, 173.2, 172.0, 171.8, 169.9, 157.3, 153.3, 142.2, 138.0, 136.3, 134.2, 133.9, 129.6, 129.5, 129.1, 128.6, 128.5, 126.9, 126.8, 124.7, 123.8, 118.2, 117.4, 115.9, 82.0, 67.4, 54.4, 52.7, 51.9, 48.8, 40.9, 37.9, 37.0, 31.3, 29.1, 27.8, 27.5, 25.5, 18.4. MS (ESI) Calculated for $C_{41}H_{56}N_{10}O_8[M+H]^+$: 816.4, found 817.2.

Acyclic-Ala-Ile-His-Phe-NH₂ (S26):



Following general procedure A, the corresponding compound was prepared from H-AIHF-NH₂ (\cdot 2TFA, 44 mg, 0.062 mmol), diisopropylethylamine (43 μ L, 0.247 mmol) and reagent 1 (25 mg, 0.062 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 20-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (34 mg, 0.044mmol, 72%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.94 (d, J = 1.6 Hz, 1H), 8.16 (d, J = 8.1 Hz, 1H), 8.04 (d, J = 7.4 Hz, 1H), 7.99 (d, J = 7.8 Hz, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.51 (br. s, 1H), 7.27-7.29 (m, 2H), 7.18-7.26 (m, 6H), 7.14-7.18 (m, 2H), 7.1 (br. d, J = 7.4 Hz, 1H), 6.62 (d, J = 16 Hz, 1H), 6.32 (dt, J = 16.0, 6.2 Hz, 1H), 4.65 (dd, J = 6.3, 1.2 Hz, 2H), 4.58 (ddd, J = 7.9, 7.9, 6.1 Hz, 1H), 4.41 (ddd, J = 8.3, 8.3, 5.1 Hz, 1H), 4.29 (dq, J = 7.0, 7.0 Hz, 1H), 4.07 (t, J = 7.6 Hz, 1H), 2.95-3.00 (m, 2H), 2.91 (dd, J = 15.4, 8.0 Hz, 1H), 2.75-2.85 (m, 3H), 2.36-2.45 (m, 2H), 1.59-1.66 (m, 1H), 1.41 (s, 9H), 1.27-1.34 (m, 1H), 1.1 (d, J = 7 Hz, 3H), 0.94-1.04 (m, 1H), 0.74 (t, J = 7.4 Hz, 3H), 0.69 (d, J = 6.7 Hz, 3H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 173.2, 172.9, 171.8, 171.4, 170.0, 153.3, 142.2, 138.0, 136.3, 134.2, 133.9, 129.6, 129.6, 129.1, 128.5, 128.5, 126.9, 126.8, 124.7, 123.8, 117.3, 82.0, 67.4, 57.4, 54.3, 51.8, 48.5, 37.9, 37.1, 36.9, 31.4, 27.8, 27.5, 24.7, 18.3, 15.7, 11.5. MS (ESI) Calculated for $C_{41}H_{55}N_7O_8[M+H]^+$: 774.4, found 774.2.

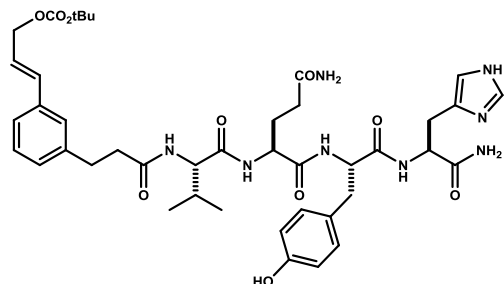
Acyclic- β -Ala-Prof[4-(2-methoxy-4-methylphenoxy)]-His (S27):



Following general procedure A, the corresponding compound was prepared from H-(β -)AP(4-OAr)H-NH₂ (\cdot 2TFA, 112 mg, 0.163 mmol), diisopropylethylamine (114 μ L, 0.653 mmol) and reagent 1 (66 mg, 0.163 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 30-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (95 mg, 0.127mmol, 78%). ¹H NMR (DMSO-d₆, 500 MHz): 5:1 mixture of rotamers. Major: δ 8.86 (d, J = 0.9 Hz, 1H), 8.14 (d, J = 8.7 Hz, 1H), 7.91 (d, J = 5.7 Hz, 1H), 7.33 (br. s, 1H), 7.25-7.31 (m, 2H), 7.17-7.24 (m, 3H), 7.06-7.10 (m, 2H), 6.75-6.82 (m, 2H), 6.64 (br. d, J = 8.3 Hz, 1H), 6.59 (d, J = 16 Hz, 1H), 6.3 (dt, J = 15.9, 6.3 Hz, 1H), 4.76-4.80 (m, 1H), 4.64 (d, J = 6.4 Hz, 2H), 4.51 (ddd, J = 9.2, 9.2, 4.6 Hz, 1H), 4.29 (dd, J = 9.9, 3.9 Hz, 1H), 3.71-3.73 (m, 1H), 3.7 (s, 3H), 3.19-3.29 (m, 3H), 2.93 (dd, J = 15.5, 9.7 Hz, 1H), 2.77 (t, J = 7.7 Hz, 2H), 2.26-2.53 (m, 6H), 2.23 (s, 3H), 1.99 (dt, J = 13.0, 3.1 Hz, 1H), 1.4

(s, 9H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 172.4, 172.0, 171.9, 171.8, 153.3, 150.6, 143.8, 142.1, 136.3, 133.9, 132.9, 130.5, 129.0, 128.6, 126.9, 124.7, 123.7, 121.3, 118.8, 116.9, 113.8, 82.0, 78.2, 67.4, 59.7, 55.9, 52.3, 51.7, 37.3, 35.1, 34.7, 31.4, 27.8, 26.5, 21.2. MS (ESI) Calculated for C₃₉H₅₀N₆O₉[M+H]⁺:747.4, found 747.3.

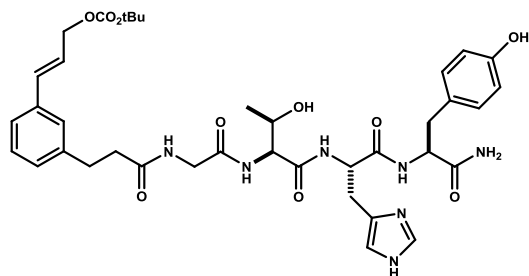
Acyclic-Val-Gln-Tyr-His-NH₂ (18):



Following general procedure A, the corresponding compound was prepared from H-VQYH-NH₂ (•2TFA, 170 mg, 0.220mmol), diisopropylethylamine (153μL, 0.88 mmol) and reagent 1 (89 mg, 0.220mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 20-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (103 mg, 0.123mmol, 56%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.94 (d, J = 1.4 Hz, 1H), 8.19 (d, J = 8.3 Hz, 1H), 8.11 (d, J = 7.3 Hz, 1H), 7.91 (d, J = 7.8 Hz, 2H), 7.32 (br. s, J = Hz, 1H), 7.18-

7.30 (m, 5H), 7.14 (br. s, J = Hz, 1H), 7.1 (br. d, J = 7.3 Hz, 1H), 6.96 (d, J = 8.4 Hz, 2H), 6.83 (br. s, J = Hz, 1H), 6.57-6.63 (m, 3H), 6.31 (dt, J = 16.0, 6.2 Hz, 1H), 4.65 (dd, J = 6.4, 1.2 Hz, 2H), 4.46 (ddd, J = 8.2, 8.2, 5.5 Hz, 1H), 4.32 (ddd, J = 8.1, 8.1, 5.0 Hz, 1H), 4.16 (ddd, J = 8.0, 8.0, 5.7 Hz, 1H), 4.04-4.09 (m, 1H), 3.1 (dd, J = 15.3, 5.2 Hz, 1H), 2.89 (dd, J = 15.4, 8.6 Hz, 1H), 2.74-2.86 (m, 3H), 2.68 (dd, J = 14.1, 9.1 Hz, 1H), 2.50-2.58 (m, 1H), 2.39-2.46 (m, 1H), 2.00-2.12 (m, 2H), 1.75-1.90 (m, 2H), 1.61-1.70 (m, 1H), 1.4 (s, 9H), 0.73 (d, J = 6.7 Hz, 6H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 174.6, 172.4, 172.0, 171.9, 171.8, 171.6, 156.3, 153.3, 142.1, 136.3, 134.1, 133.9, 130.4, 129.9, 129.1, 128.5, 127.9, 126.8, 124.7, 123.7, 117.3, 115.4, 82.0, 67.4, 58.6, 55.0, 52.7, 51.9, 37.0, 31.8, 31.5, 30.7, 28.1, 27.8, 27.3, 19.6, 18.7. MS (ESI) Calculated for C₄₂H₅₆N₈O₁₀[M+H]⁺:833.4, found 833.2.

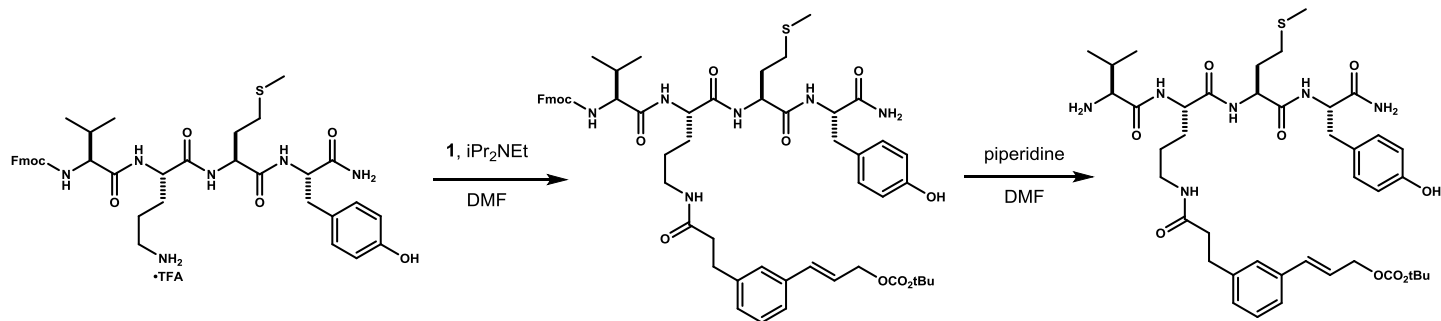
Acyclic-Gly-Thr-His-Tyr-NH₂ (S29):



Following general procedure A, the corresponding compound was prepared from H-GTHY-NH₂ (•2TFA, 37 mg, 0.053 mmol), diisopropylethylamine (37 μL, 0.210 mmol) and reagent 1 (21 mg, 0.053 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 20-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (27 mg, 0.036mmol, 68%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.92 (d, J = 1.4 Hz, H), 8.2 (t, J = 5.9 Hz, H), 8.15 (d, J = 8 Hz, H), 7.95 (d, J = 7.8 Hz, H), 7.8 (d, J = 8 Hz, H), 7.44

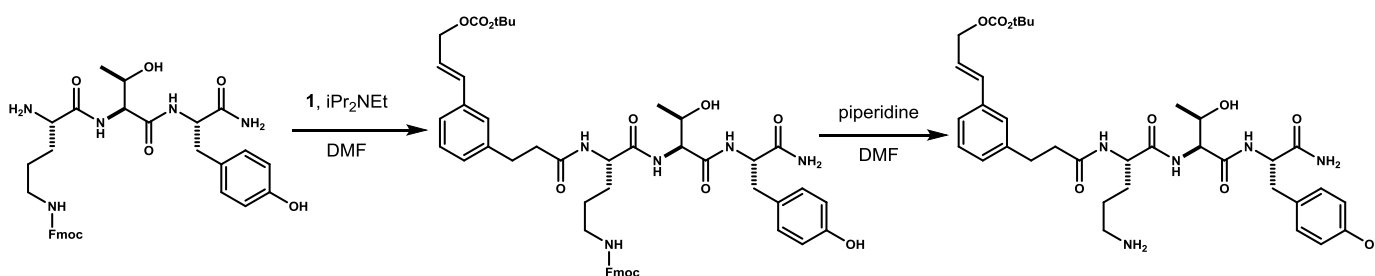
(br. s, H), 7.24-7.30 (m, H), 7.22 (t, J = 7.5 Hz, H), 7.15 (br. s, H), 7.1 (br. d, J = 7.3 Hz, H), 7.01 (d, J = 8.5 Hz, H), 6.59-6.65 (m, H), 6.32 (dt, J = 16.1, 6.3 Hz, H), 4.65 (dd, J = 6.3m 1.1 Hz, H), 4.54 (ddd, J = 8.0, 8.0, 5.4 Hz, H), 4.3 (ddd, J = 8.3, 8.3, 5.2 Hz, H), 4.19 (dd, J = 8.0, 4.5 Hz, H), 3.94 (dddd, J = 6.5, 6.5, 6.5, 4.7 Hz, H), 3.71-3.81 (m, H), 3.06 (dd, J = 15.3, 5.1 Hz, H), 2.93 (dd, J = 15.3, 8.3 Hz, H), 2.87 (dd, J = 13.7, 4.9 Hz, H), 2.76-2.81 (m, H), 2.69 (dd, J = 14.0, 8.9 Hz, H), 2.40-2.47 (m, H), 1.41 (s, H), 0.99 (d, J = 6.4 Hz, H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 173.6, 172.5, 170.5, 170.0, 169.9, 156.3, 153.3, 142.2, 136.4, 134.2, 133.9, 130.5, 129.6, 129.1, 128.5, 128.1, 126.9, 124.7, 123.8, 117.5, 115.4, 82.0, 67.4, 66.9, 58.6, 55.0, 52.1, 42.6, 37.1, 31.8, 31.3, 27.8, 27.2, 20.0. MS (ESI) Calculated for C₃₈H₄₉N₇O₁₀ [M+H]⁺: 764.4, found 764.1.

Acyclic-Val-Orn-Met-Tyr (S30):



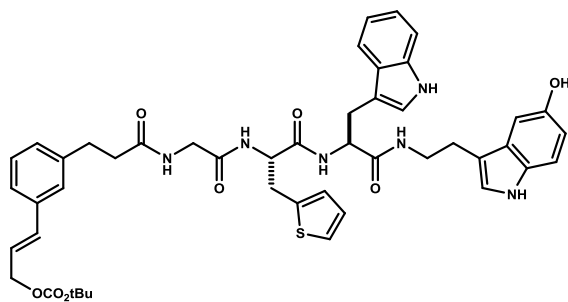
Following general procedure A, the corresponding compound was prepared from Fmoc-VOMY-NH₂ (*1TFA, 94 mg, 0.110mmol), diisopropylethylamine (76μL, 0.440mmol) and reagent 1 (22 mg, 0.110mmol). The reaction mixture was evaporated under reduced pressure. The resulting residue was treated with 20% piperidine/DMF (8 ml) for two hours and evaporated. The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 30-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (56 mg, 0.069 mmol, 62%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.49 (d, J = 7.7 Hz, 1H), 8.14 (d, J = 8.4 Hz, 1H), 8.03-8.09 (m, 3H), 7.84 (dd, J = 5.7, 5.7 Hz, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.4 (br. s, J = Hz, 1H), 7.19-7.29 (m, 3H), 7.09 (br. d, J = 7.4 Hz, 1H), 7.05 (br. s, J = Hz, 1H), 6.98 (d, J = 8.6 Hz, 2H), 6.58-6.64 (m, 3H), 6.31 (dt, J = 15.9, 6.3 Hz, 1H), 4.65 (dd, J = 6.3, 1.2 Hz, 2H), 4.25-4.37 (m, 3H), 3.56-3.62 (m, 1H), 2.96-3.09 (m, 2H), 2.84 (dd, J = 13.9, 5.2 Hz, 1H), 2.75-2.80 (m, 2H), 2.68 (dd, J = 14.1, 8.6 Hz, 1H), 2.30-2.42 (m, 4H), 1.96-2.06 (m, 4H), 1.80-1.89 (m, 1H), 1.67-1.76 (m, 1H), 1.55-1.64 (m, 1H), 1.31-1.51 (m, 12H), 0.9 (d, J = 2.4 Hz, 3H), 0.89 (d, J = 2.7 Hz, 3H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 173.3, 171.8, 171.5, 170.9, 168.2, 156.3, 153.3, 142.3, 136.3, 133.9, 130.6, 129.1, 128.5, 128.1, 126.9, 124.7, 123.8, 115.3, 82.0, 67.4, 57.6, 54.4, 52.8, 52.5, 38.5, 37.5, 37.3, 32.6, 31.5, 30.4, 29.8, 27.8, 18.7, 18.1, 15.0. MS (ESI) Calculated for C₄₁H₆₀N₆O₉S [M+H]⁺: 813.4, found 813.2.

Acyclic-Orn-Thr-Tyr (S35):



Following general procedure A, the corresponding compound was prepared from Orn(Fmoc)-Thr-Tyr-NH₂ (*1TFA, 109 mg, 0.15mmol), diisopropylethylamine (52μL, 0.30mmol) and reagent 1 (60 mg, 0.15mmol). The reaction mixture was evaporated under reduced pressure. The resulting residue was treated with DBU (1 equiv.) and Si-Thiol (Silicycle, 1.22 g/mmol) in DMF (1 ml) for one hour. The product was filtered and purified by preparative HPLC (Waters Xbridge C18 19x250 mm) using a gradient of 30-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and evaporated (116 mg, 0.145mmol, 97%). ¹H NMR (DMSO-d₆, 500 MHz): δ 9.20 (br s, 1H), 8.14 (d, J = 8.2 Hz, 1H), 7.86 (d, J = 8.3 Hz, 1H), 7.71 (d, J = 8.2 Hz, 1H), 7.65-7.70 (m, 3H), 7.42 (br s, 1H), 7.30 (br s, 1H), 7.27 (br d, J = 7.6 Hz, 1H), 7.24 (dd, J = 7.6, 7.3 Hz, 1H), 7.16 (br s, 1H), 7.11 (br d, J = 7.3 Hz, 1H), 7.01 (d, J = 8.4 Hz, 2H), 6.64 (d, J = 15.9 Hz, 1H), 6.63 (d, J = 8.4 Hz, 2H), 6.34 (dt, J = 15.9, 6.2 Hz, 1H), 4.67 (d, J = 6.1 Hz, 2H), 4.38-4.43 (m, 1H), 4.36 (ddd, J = 8.1, 8.0, 5.3 Hz, 1H), 4.18 (dd, J = 8.2, 4.2 Hz, 1H), 3.96-4.02 (m, 1H), 2.91 (dd, J = 14.0, 5.0 Hz, 1H), 2.80 (dd, J = 9.0, 6.8 Hz, 2H), 2.66-2.78 (m, 3H), 2.45 (dd, J = 8.3, 6.8 Hz, 2H), 1.63-1.72 (m, 1H), 1.46-1.54 (m, 3H), 1.43 (s, 9H), 0.97 (d, J = 6.3 Hz, 3H). ¹³C NMR (DMSO-d₆, 100 MHz): δ 173.1, 171.6, 169.4, 155.8, 152.8, 141.7, 135.9, 133.4, 130.1, 128.7, 128.0, 127.7, 126.4, 124.3, 123.4, 114.9, 81.6, 66.9, 66.4, 58.1, 54.1, 51.6, 38.5, 36.7, 31.0, 28.8, 27.4, 23.5, 19.4. MS (ESI) Calculated for C₃₅H₄₅N₅O₉ [M+H]⁺: 684.4, found 684.2.

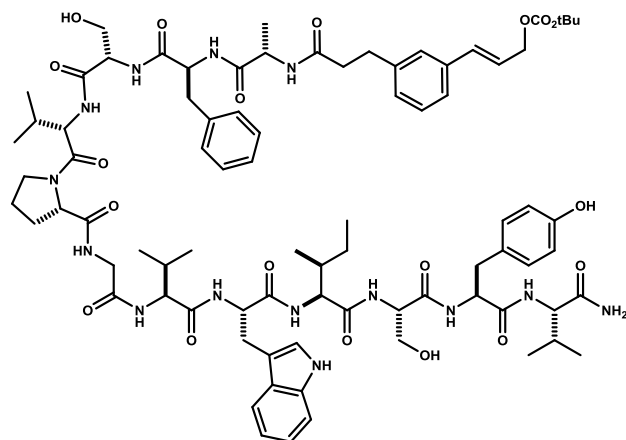
Acyclic-Gly-Thi-Trp-5HT (S31):



Following general procedure A, the corresponding compound was prepared from H-GThiW-5HT-NH₂ (*TFA, 52 mg, 0.091 mmol), diisopropylethylamine (63 μL, 0.363 mmol) and reagent 1 (37 mg, 0.091 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (45 mg, 0.052mmol, 57%). ¹H NMR (DMSO-d₆, 600 MHz): δ 10.75 (s, 1H), 10.42 (s, 1H), 8.08-8.14 (m, 2H), 7.85 (t, J = 5.6 Hz, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.30 (d, J = 8.1 Hz, 1H), 7.22-7.27 (m, 3H), 7.20 (t, J = 7.5 Hz, 1H), 7.06-7.11 (m, 3H), 7.02 (dd, J = 7.4, 7.4 Hz, 1H), 6.96-6.98 (m, 1H), 6.94 (dd, J = 7.4, 7.4 Hz, 1H), 6.85 (dd, J = 4.7, 4.0 Hz, 1H), 6.80-6.83

(m, 2H), 6.59 (d, J = 16.2 Hz, 1H), 6.57 (dd, J = 8.6, 2.2 Hz, 1H), 6.29 (dt, J = 16.0, 6.3 Hz, 1H), 4.63 (d, J = 6.4 Hz, 2H), 4.44-4.52 (m, 2H), 3.74 (dd, J = 16.5, 5.7 Hz, 1H), 3.62 (dd, J = 16.3, 5.6 Hz, 1H), 3.21-3.27 (m, 2H), 3.18 (dd, J = 15.1, 4.3 Hz, 1H), 3.11 (dd, J = 14.5, 5.4 Hz, 1H), 2.96-3.01 (m, 2H), 2.78 (t, J = 7.7 Hz, 1H), 2.62 (t, 7.7 Hz, 1H), 2.40-2.45 (m, 2H), 1.40 (s, 9H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 172.3, 171.2, 170.4, 169.5, 153.1, 150.5, 142.1, 139.7, 136.4, 136.2, 133.7, 131.1, 129.0, 128.3, 128.1, 127.7, 127.0, 126.8, 126.6, 124.8, 124.5, 123.9, 123.7, 123.4, 121.2, 118.8, 118.6, 112.0, 111.60, 111.57, 111.0, 110.3, 102.5, 81.8, 67.2, 54.2, 54.1, 42.4, 37.0, 31.9. MS (ESI) Calculated for C₄₇H₅₂N₆O₈S [M+H]⁺: 861.4, found 861.3.

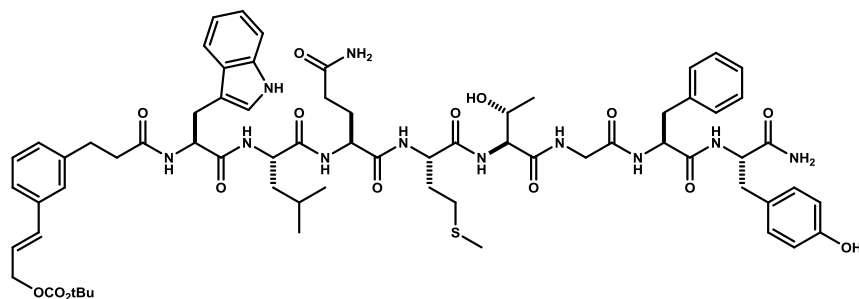
Acyclic-Ala-Phe-Ser-Val-Pro-Gly-Val-Trp-Ile-Ser-Tyr-Val (S32):



Following general procedure A, the corresponding compound was prepared from H-AFSVPGVWISYV-NH₂ (•TFA, 75 mg, 0.052 mmol), diisopropylethylamine (36 μL, 0.209 mmol) and reagent 1 (21 mg, 0.052 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 30-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (61 mg, 0.038mmol, 72%). ¹H NMR (DMSO-d₆, 600 MHz): δ 10.68 (s, 1H), 8.18 (d, J = 8 Hz, 1H), 8.09 (dd, J = 5.6 Hz, 1H), 8.02 (d, J = 7.6 Hz, 1H), 7.91-7.98 (m, 3H), 7.89 (d, J = 8.1 Hz, 1H), 7.84 (d, J = 8.7 Hz, 1H), 7.79 (d, J = 8.7 Hz, 1H), 7.71 (d, J = 9.1 Hz, 1H), 7.56 (d, J = 8.9 Hz, 1H), 7.53 (d, J = 8.2 Hz, 1H), 7.16-7.28 (m, 9H), 7.10-7.15 (m, 1H), 7.04-7.09 (m, 3H), 7 (t,

J = 7.4 Hz, 1H), 6.96 (d, J = 8.3 Hz, 2H), 6.92 (t, J = 7.5 Hz, 1H), 6.6 (d, J = 16 Hz, 1H), 6.56 (d, J = 8.1 Hz, 2H), 6.3 (dt, J = 16.0, 6.3 Hz, 1H), 4.63 (d, J = 6.1 Hz, 2H), 4.55 (ddd, J = 8.4, 8.4, 8.4 Hz, 1H), 4.63 (ddd, J = 8.7, 8.7, 4.2 Hz, 1H), 6.06 (ddd, J = 8.0, 8.0, 5.0 Hz, 1H), 4.12-4.36 (m, 4H), 4.14-4.23 (m, 3H), 4.06 (dd, J = 8.8, 6.7 Hz, 1H), 3.71 (dd, J = 16.5, 5.8 Hz, 1H), 3.61-3.66 (m, 1H), 3.44-3.60 (m, 5H), 3.06 (dd, J = 14.3, 3.9 Hz, 1H), 3.01 (dd, J = 13.9, 3.7 Hz, 1H), 2.84-2.93 (m, 2H), 2.67-2.79 (m, 4H), 1.84-2.03 (m, 5H), 1.73-1.81 (m, 2H), 1.61-1.69 (m, 1H), 1.39 (s, 9H), 1.32-1.38 (m, 1H), 1.04 (d, J = 7 Hz, 3H), 0.96-1.03 (m, 1H), 0.87 (d, J = 6.4 Hz, 3H), 0.70-0.83 (m, 21H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.1, 172.4, 172.3, 171.64, 171.56, 171.1, 171.03, 171.00, 170.9, 170.2, 170.05, 170.01, 168.8, 156.1, 153.1, 142.0, 138.0, 136.3, 136.2, 133.8, 130.3, 129.6, 128.9, 128.34, 128.26, 127.9, 127.6, 126.7, 126.5, 124.6, 123.9, 123.7, 121.1, 118.7, 118.5, 115.2, 111.5, 110.3, 81.8, 67.2, 62.1, 62.0, 59.89, 57.90, 57.7, 57.1, 56.0, 55.3, 55.2, 54.7, 53.9, 53.7, 48.6, 47.4, 42.4, 37.6, 37.2, 36.9, 36.6, 31.1, 31.0, 30.7, 30.4, 29.5, 27.7, 24.7, 24.5, 19.6, 19.6, 19.5, 18.4, 18.2. MS (ESI) Calculated for C₈₃H₁₁₄N₁₄O₁₉[M+2H]²⁺: 806.4, found 806.2.

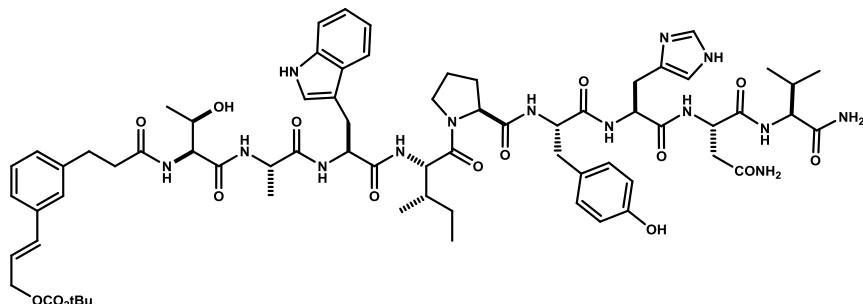
Acyclic-Trp-Leu-Gln-Met-Thr-Gly-Phe-Tyr (S33):



Following general procedure A, the corresponding compound was prepared from H-WLQMTGFY-NH₂ (•TFA, 83 mg, 0.072 mmol), diisopropylethylamine (50 μL, 0.287 mmol) and reagent 1 (29 mg, 0.072mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 40-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (61 mg, 0.046mmol, 64%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.74 (d, J = 1.6 Hz, 1H), 7.97-8.10 (m, 7H), 7.73 (d, J = 8.1 Hz, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.29 (d, J = 8.2 Hz, 1H), 7.11-7.26 (m, 10H), 7.08 (d, J = 2.6 Hz, 1H), 6.97-7.05 (m, 5H), 6.95 (t, J = 7.9 Hz, 1H), 6.78 (br. s, J = Hz, 1H), 6.62 (d, J = 8.4 Hz, 2H), 6.58 (d, J = 16.1 Hz, 1H), 6.3 (dt, J = 16.1, 6.2 Hz, 1H), 4.64 (dd, J = 6.3, 1.1 Hz, 2H), 4.55 (ddd, J = 8.6, 8.6, 4.6 Hz, 1H), 4.46 (ddd, J = 8.7, 8.7, 4.7 Hz, 1H), 4.41 (ddd, J = 8.4, 8.4, 4.8 Hz, 1H), 4.27-4.33 (m, 2H), 4.23 (dq, J = 7.7, 7.7 Hz, 1H), 4.18 (dd, J = 8.0, 3.9 Hz, 1H), 3.91-3.97 (m, 1H), 3.68 (dd, J = 17.0, 5.4 Hz, 1H), 3.62 (dd, J = 16.7, 5.2 Hz, 1H), 3.08 (dd, J = 14.6, 4.2 Hz, 1H), 2.93 (dd, J = 13.7, 4.4 Hz, 1H), 2.83-2.91 (m, 2H), 2.60-2.72 (m, 4H), 2.30-2.46 (m, 4H), 2.06-

2.13 (m, 2H), 1.98 (s, 3H), 1.81-1.96 (m, 2H), 1.70-1.81 (m, 2H), 1.49-1.61 (m, 1H), 1.36-1.46 (m, 11H), 0.85 (d, J = 6.4 Hz, 3H), 0.81 (d, J = 6.6 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 174.3, 173.3, 172.4, 172.1, 171.8, 171.7, 171.6, 171.0, 170.7, 169.0, 156.2, 153.3, 142.2, 138.1, 136.5, 136.3, 133.9, 130.6, 129.7, 129.1, 128.5, 128.4, 128.3, 127.9, 126.9, 126.7, 124.6, 124.1, 123.7, 121.2, 119.0, 118.6, 115.3, 111.7, 110.6, 82.0, 67.4, 67.1, 58.7, 54.7, 54.5, 53.7, 52.6, 52.3, 51.5, 42.4, 41.3, 38.0, 37.3, 37.3, 32.2, 31.9, 31.4, 30.0, 28.2, 28.1, 27.8, 24.6, 23.5, 22.2, 20.0, 15.1. MS (ESI) Calculated for C₆₈H₈₉N₁₁O₁₅S [M+H]⁺: 1332.6, found 1332.2.

Acyclic-Thr-Ala-Trp-Ile-Pro-Tyr-His-Asn-Val (S34):

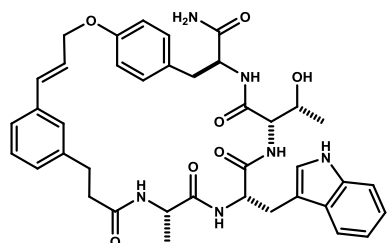


Following general procedure A, the corresponding compound was prepared from H-TAWIPYHNV-NH₂ (*2TFA, 196 mg, 0.148 mmol), diisopropylethylamine (103 μL, 0.591 mmol) and reagent 1 (60 mg, 0.148 mmol). The product was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 30-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected

were combined and lyophilized (131 mg, 0.095 mmol, 64%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.76 (s, 1H), 8.92 (s, 1H), 8.31 (d, J = 7.1 Hz, 1H), 8.18 (d, J = 7.7 Hz, 1H), 7.89-7.98 (m, 2H), 7.84 (d, J = 7.2 Hz, 1H), 7.77-7.81 (m, 2H), 7.47 (d, J = 7.9 Hz, 1H), 7.44 (s, 1H), 7.38 (s, 1H), 7.33 (s, 1H), 7.25-7.29 (m, 2H), 7.16-7.24 (m, 2H), 7.04-7.09 (m, 3H), 6.90-7.03 (m, 4H), 6.91 (d, J = 7.3 Hz, 1H), 6.56-6.62 (m, 3H), 6.29 (dt, J = 15.8, 6.2 Hz, 1H), 4.63 (dd, J = 6.2, 0.9 Hz, 2H), 4.49-4.61 (m, 3H), 4.18-4.32 (m, 5H), 4.04-4.08 (m, 1H), 3.9 (ddd, J = 10.0, 10.0, 5.7 Hz, 1H), 3.50-3.56 (m, 1H), 3.41-3.47 (m, 1H), 3.00-3.10 (m, 2H), 2.86-2.97 (m, 2H), 2.75-2.82 (m, 2H), 2.41-2.57 (m, 5H), 2 (dq, J = 13.5, 6.8 Hz, 1H), 1.82-1.91 (m, 1H), 1.59-1.75 (m, 4H), 1.41-1.48 (m, 1H), 1.39 (s, 9H), 0.92 (d, J = 6.2 Hz, 3H), 0.71-0.81 (m, 12H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.0, 172.2, 172.0, 171.9, 171.5, 171.3, 171.2, 170.3, 170.2, 169.8, 161.8, 156.1, 153.1, 142.0, 136.3, 136.1, 134.0, 133.8, 130.3, 129.3, 128.9, 128.4, 128.0, 127.7, 126.7, 124.5, 123.9, 123.6, 121.1, 118.7, 118.5, 117.3, 116.7, 115.2, 114.8, 112.9, 111.5, 110.0, 81.8, 67.2, 66.9, 59.6, 58.3, 57.9, 54.9, 53.5, 51.6, 50.3, 48.6, 37.1, 36.9, 36.4, 31.3, 30.4, 29.2, 27.7, 24.5, 24.4, 24.3, 19.8, 19.6, 18.4, 17.8, 15.3, 11.1. MS (ESI) Calculated for C₇₀H₉₄N₁₄O₁₆ [M+H]⁺: 1387.7, found 1387.4.

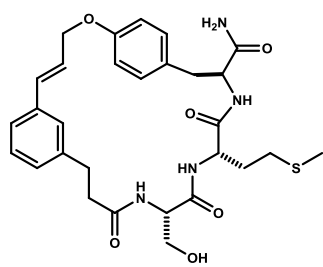
Data for macrocyclic compounds:

Cyclic-Ala-Trp-Thr-Tyr (4):



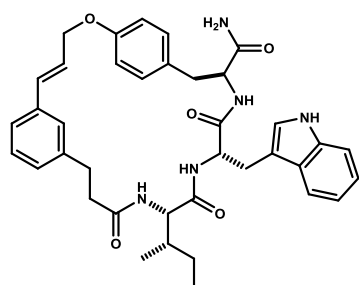
Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (8 mg, 0.011 mmol, 78%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.81 (d, J = 1.8 Hz, 1H), 8.1 (d, J = 7.5 Hz, 1H), 8.01 (d, J = 7.4 Hz, 1H), 7.68 (d, J = 8.1 Hz, 1H), 7.51 (d, J = 8.1 Hz, 1H), 7.25-7.36 (m, 3H), 7.06-7.22 (m, 5H), 6.89-7.05 (m, 3H), 6.79 (d, J = 8.7 Hz, 2H), 6.61 (d, J = 8.3 Hz, 2H), 6.53 (d, J = 15.9 Hz, 1H), 2.28 (dt, J = 16.0, 5.7 Hz, 1H), 4.15 (d, J = 5.4 Hz, 2H), 4.31-4.42 (m, 3H), 4.07-4.14 (m, 1H), 3.91-3.99 (m, 1H), 2.86-3.16 (m, 4H), 2.65-2.80 (m, 3H), 2.23-3.38 (m, 1H), 0.94 (d, J = 7.5 Hz, 3H), 0.86 (d, J = 6.4 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.6, 173.4, 172.9, 172.1, 169.9, 156.2, 141.8, 136.5, 132.7, 130.4, 130.3, 128.9, 128.5, 128.3, 127.8, 126.0, 125.7, 124.8, 124.2, 121.3, 118.7, 115.4, 115.1, 111.8, 110.2, 68.2, 67.0, 66.6, 58.4, 54.6, 49.0, 36.1, 30.7, 27.5, 19.5, 18.1. MS (ESI) Calculated for C₃₉H₄₄N₆O₇ [M+H]⁺: 709.3, found 709.0.

Cyclic-Ser-Met-Tyr (5):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (15 mg, 0.026mmol, 80%). ¹H NMR (DMSO-d₆, 600 MHz): δ 7.96 (d, J = 8.2 Hz, 1H), 7.92 (d, J = 7.9 Hz, 1H), 7.75 (d, J = 7.9 Hz, 1H), 7.37 (s, 1H), 7.24 (s, 1H), 7.13-7.21 (m, 2H), 7.04-7.11 (m, 3H), 7.00 (d, J = 8.1 Hz, 1H), 6.81 (d, J = 8.46 Hz, 2H), 6.60 (d, J = 15.9, 1H), 6.36 (dt, J = 16.1, 5.7 Hz, 1H), 4.77 (d, J = 5.5 Hz, 2H), 4.21-4.31 (m, 2H), 4.14 (ddd, J = 6.9, 6.9, 6.9 Hz, 1H), 3.12 (dd, J = 10.6, 5.3 Hz, 1H), 3.06 (d, J = 10.9, 6.9 Hz, 1H), 2.89 (app d, J = 14.2 Hz, 1H), 2.68-2.84 (m, 3H), 2.55-2.64 (m, 1H), 2.27-2.39 (m, 3H), 1.96 (s, 1H), 1.74-1.82 (m, 1H), 1.58-1.66 (m, 1H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.3, 171.8, 171.2, 170.2, 156.8, 141.4, 136.2, 132.8, 130.3, 130.0, 128.8, 128.6, 126.0, 125.6, 124.5, 115.0, 68.0, 62.2, 54.7, 54.1, 52.1, 36.4, 35.3, 31.9, 30.7, 29.7, 14.9. MS (ESI) Calculated for C₂₉H₃₆N₄O₆S [M+H]⁺: 569.2, found 569.2.

Cyclic-Ile-Trp-Tyr (6):

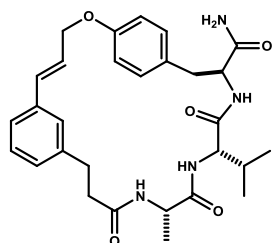


Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (12 mg, 0.019 mmol, 72%).

¹H NMR (DMSO-d₆, 500 MHz): 10.8 (d, J = 1.8 Hz, 1H), 7.81 (d, J = 8.3 Hz, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.52 (br. s, J = Hz, 1H), 7.36 (d, J = 8.5 Hz, 1H), 7.31 (br. d, J = 7.9 Hz, 1H), 7.19 (br. s, J = Hz, 1H), 7.09-7.06 (m, 3H), 6.92-7.07 (m, 6H), 6.8 (d, J = 8.7 Hz, 2H), 6.68 (d, J = 16 Hz, 1H), 6.51 (dt, J = 15.8, 6.4 Hz, 1H), 4.66-4.77 (m, 2H), 4.54 (ddd, J = 8.3, 8.3, 5.6 Hz, 1H), 4.24 (ddd, J = 8.2, 8.2, 4.8 Hz, 1H), 3.84 (app. dd, J = 8.0, 6.9 Hz, 1H), 2.95 (ddd, J = 15.0, 5.4 Hz, 1H), 2.68-2.90 (m, 6H), 2.27-2.35 (m, 1H), 1.11-1.19 (m, 1H), 0.57-0.71 (m, 2H), 0.26-0.31 (m, 3H), 0.08 (d, J = 6.7 Hz, 3H).

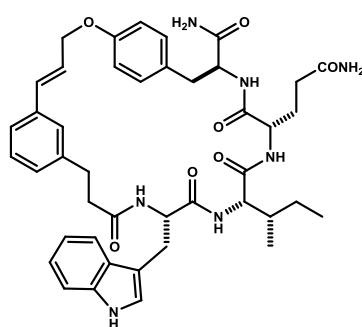
¹³C NMR (DMSO-d₆, 125 MHz): δ 173.9, 171.6, 171.4, 170.9, 157.2, 140.9, 136.7, 136.5, 134.3, 130.6, 129.9, 129.1, 128.7, 127.7, 125.8, 125.6, 125.3, 124.2, 121.3, 119.0, 118.6, 114.7, 111.8, 110.4, 68.5, 56.8, 54.6, 53.0, 38.2, 36.7, 34.9, 30.9, 27.1, 23.8, 15.1, 11.3. MS (ESI) Calculated for C₃₈H₄₃N₅O₅ [M+H]⁺: 650.3, found 650.0

Cyclic-Ala-Val-Tyr (7):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (10 mg, 0.020mmol, 78%). ¹H NMR (DMSO-d₆, 600 MHz): δ 7.82 (d, J = 8.9 Hz, 1H), 7.69 (d, J = 8.8 Hz, 1H), 7.52 (d, J = 7.1 Hz, 1H), 7.22 (s, 1H), 7.15-7.20 (m, 3H), 7.08 (s, 1H), 7.00-7.05 (m, 3H), 6.78 (d, J = 8.5 Hz, 2H), 6.64 (d, J = 16.0 Hz, 1H), 6.31 (dt, J = 15.8, 6.0 Hz, 1H), 4.74 (d, J = 5.8 Hz, 2H), 5.82 (ddd, J = 9.8, 9.8, 2.9 Hz, 1H), 4.74 (dq, J = 7.0, 7.0 Hz, 1H), 3.93 (dd, J = 8.6, 8.6 Hz, 1H), 2.81-2.89 (m, 2H), 2.71-2.79 (m, 2H), 2.53-2.60 (m, 1H), 2.21-2.27 (m, 1H), 1.81 (dddd, J = 13.5, 6.5, 6.5, 6.5 Hz, 1H), 1.38 (d, J = 6.8 Hz, 3H), 0.63 (d, J = 6.6 Hz, 6H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.5, 172.2, 171.3, 170.9, 157.0, 141.4, 136.0, 133.2, 130.0, 129.7, 128.8, 128.8, 125.9, 125.0, 114.9, 68.2, 58.4, 53.3, 47.9, 36.4, 35.8, 31.1, 29.9, 19.5, 19.4, 18.4. MS (ESI) Calculated for C₂₉H₃₆N₄O₅[M+H]⁺: 521.3, found 521.2.

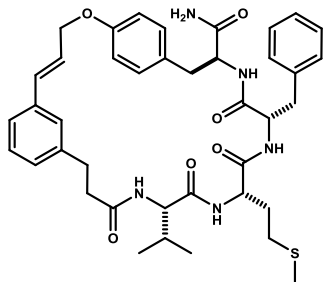
Cyclic-Trp-Ile-Gln-Tyr (8):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (11 mg, 0.014 mmol, 81%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.76 (d, J = 1.9 Hz, 1H), 8.22 (d, J = 7.8 Hz, 1H), 7.83 (d, J = 7.5 Hz, 1H), 7.79 (d, J = 7.8 Hz, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.37 (br. s, 1H), 7.27-7.34 (m, 2H), 7.16-7.25 (m, 3H), 7.08-

7.15 (m, 3H), 6.99-7.08 (m, 4H), 6.95 (t, J = 7.4 Hz, 1H), 6.81 (d, J = 8.7 Hz, 2H), 6.73 (br. s, 1H), 6.61 (d, J = 16 Hz, 1H), 6.35 (dt, J = 15.9, 5.6 Hz, 1H), 4.69-4.79 (m, 2H), 4.38 (ddd, J = 9.6, 7.8, 4.4 Hz, 1H), 4.32 (ddd, J = 10.8, 7.7, 3.1 Hz, 1H), 4.2 (dd, J = 8.0, 5.7 Hz, 1H), 4.12 (ddd, J = 7.9, 7.9, 5.1 Hz, 1H), 3.14 (dd, J = 15.0, 4.3 Hz, 1H), 2.85-2.96 (m, 2H), 2.74-2.83 (m, 1H), 2.63-2.74 (m, 2H), 2.30-2.41 (m, 2H), 1.99-2.15 (m, 1H), 1.78-1.93 (m, 1H), 1.57-1.73 (m, 2H), 1.17-1.31 (m, 1H), 0.89-1.01 (m, 1H), 0.64-0.74 (m, 6H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 174.3, 174.0, 172.5, 171.83, 171.81, 170.8, 157.0, 142.2, 136.6, 136.5, 132.7, 130.4, 130.2, 129.0, 128.1, 127.7, 126.6, 125.6, 124.7, 123.7, 121.4, 118.8, 118.7, 115.0, 111.8, 110.9, 68.1, 56.6, 54.8, 54.6, 52.6, 37.8, 36.9, 36.7, 32.0, 30.9, 28.0, 27.5, 24.5, 15.6, 11.8. MS (ESI) Calculated for C₄₃H₅₁N₇O₇ [M+H]⁺: 778.4, found 778.0.

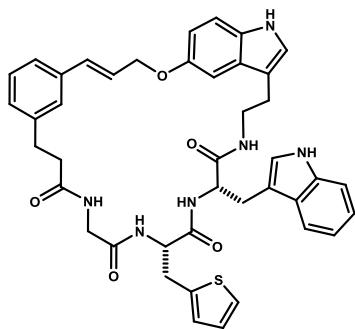
Cyclic-Val-Met-Phe-Tyr (9):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (9 mg, 0.012mmol, 73%). ¹H NMR (DMSO-d₆, 600 MHz): δ 8.24 (d, J = 8.6 Hz, 1H), 8.04 (d, J = 7.0 Hz, 1H), 7.82 (d, J = 8.9 Hz, 1H), 7.39-7.43 (m, 2H), 7.09-7.22 (m, 11H), 7.01 (d, J = 6.7 Hz, 1H), 6.82 (d, J = 8.7 Hz, 2H), 6.72 (d, J = 15.7 Hz, 1H), 6.53 (ddd, J = 16.0, 6.6, 4.9 Hz, 1H), 4.74-4.85 (m, 2H), 4.32-4.41 (m, 2H), 4.09-4.16 (m, 2H), 3.13 (dd, J = 13.8, 4.8 Hz, 1H), 2.94 (dd, J = 14.0, 2.5 Hz, 1H), 2.77-2.85 (m, 4H), 2.65 (dd, J = 13.9, 11.6 Hz, 1H), 2.26-2.40 (m, 3H), 1.97 (s, 3H), 1.66-2.04 (m, 3H), 0.254 (d, J = 6.9 Hz, 3H), 0.17 (d, J = 6.7 Hz, 3H). ¹³C NMR (DMSO-d₆, 100 MHz): δ

173.5, 171.5, 171.4, 170.8, 170.1, 156.7, 140.8, 137.0, 136.2, 132.3, 130.0, 129.8, 129.5, 128.5, 128.2, 127.8, 126.2, 125.7, 124.9, 124.6, 114.2, 67.8, 56.7, 54.6, 53.0, 52.4, 48.6, 36.9, 36.8, 34.8, 31.1, 30.4, 29.3, 18.7, 16.2, 14.4. MS (ESI) Calculated for C₄₀H₄₉N₅O₆S [M+H]⁺: 728.3, found 728.2.

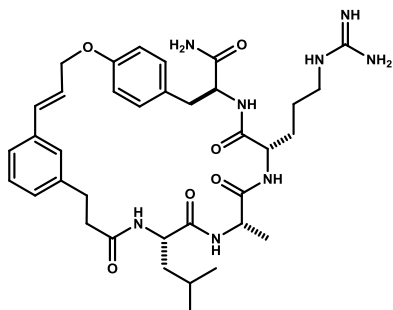
Cyclic-Gly-Thi-Trp-5HT (10):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (16 mg, 0.021 mmol, 69%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.79 (s, 1H), 10.60 (s, 1H), 8.57 (d, J = 7.6 Hz, 1H), 8.47 (t, J = 5.5 Hz, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.81 (t, J = 5.9 Hz, 1H), 7.53-7.56 (m, 2H), 7.48 (d, J = 7.9 Hz, 1H), 7.46 (d, J = 7.9 Hz, 1H), 7.32-7.37 (m, 2H), 7.30 (d, J = 7.7 Hz, 1H), 7.23-7.27 (m, 2H), 7.22 (d, J = 7.7 Hz, 1H), 7.19 (d, J = 2.0 Hz, 1H), 7.15-7.18 (m, 2H), 7.10 (d, J = 1.9 Hz, 1H), 7.03 (d, J = 1.9 Hz, 1H), 7.03 (d, J = 7.9 Hz, 2H), 6.96 (dd, J = 7.4, 7.4 Hz, 1H), 6.84 (dd, J = 5.0, 3.3 Hz, 1H), 6.78-6.80 (m, 1H), 6.76 (d, J = 16.1 Hz, 1H), 6.71 (dd, J = 8.7, 2.3 Hz, 1H), 6.38 (dt, J = 16.0, 6.1 Hz, 1H), 4.52 (ddd, J

= 9.2, 9.2, 4.6 Hz, 1H), 4.28 (ddd, J = 10.5, 7.6, 3.7 Hz, 1H), 3.82 (dd, J = 15.8, 5.4 Hz, 1H), 3.49 (dd, J = 15.7, 5.8 Hz, 1H), 3.42-3.46 (m, 1H), 3.30 (dd, J = 14.6, 4.7 Hz, 1H), 3.08-3.16 (m, 2H), 2.99-3.07 (m, 1H), 2.87-2.95 (m, 2H), 2.75 (ddd, J = 14.5, 10.6, 5.2 Hz, 1H), 2.65-2.71 (m, 1H), 2.62 (ddd, J = 15.3, 10.5, 5.8 Hz, 1H), 2.28 (ddd, J = 15.4, 8.4, 6.6 Hz, 1H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.4, 171.4, 170.5, 151.4, 142.5, 140.1, 137.0, 136.5, 133.8, 132.0, 129.0, 128.3, 127.84, 127.80, 127.3, 127.1, 126.7, 126.1, 125.0, 123.9, 123.8, 121.4, 121.3, 118.83, 118.77, 112.8, 112.5, 111.84, 111.77, 110.9, 103.7, 68.9, 55.9, 54.3, 43.4, 36.9, 31.3, 30.5, 27.8. MS (ESI) Calculated for C₄₂H₄₂N₆O₅S [M+H]⁺: 743.3, found 743.2.

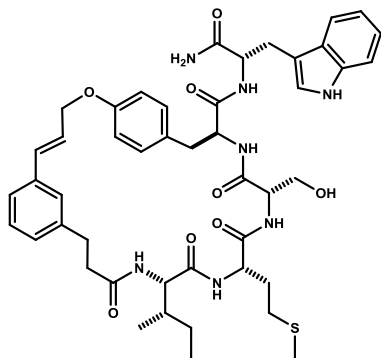
Cyclic-Ile-Ala-Arg-Tyr (11):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (13 mg, 0.019mmol, 84%). ¹H NMR (DMSO-d₆, 600 MHz): δ 8.01 (d, J = 7.4 Hz, 1H), 7.83 (d, J = 7.0 Hz, 1H), 7.72 (d, J = 8.1 Hz, 1H), 7.62 (d, J = 7.1 Hz, 1H), 7.44 (dd, J = 5.8, 5.8 Hz, 1H), 7.31 (br s, 1H), 7.21-7.25 (m, 1H), 7.19 (dd, J = 7.5, 7.5 Hz, 1H), 7.07-7.12 (m, 4H), 7.05 (d, J = 7.6 Hz, 1H), 6.81 (d, J = 8.5 Hz, 2H), 6.60 (d,

J = 16.3 Hz, 1H), 6.34 (dt, J = 16.1, 5.4 Hz, 1H), 4.71 (d, J = 5.3 Hz, 2H), 4.35 (ddd, J = 11.2, 8.3, 3.0 Hz, 1H), 4.05-4.15 (m, 3H), 2.96-3.03 (m, 3H), 2.85 (ddd, J = 13.8, 7.1, 7.1 Hz, 1H), 2.72 (ddd, J = 13.8, 6.8, 6.8 Hz, 1H), 2.64 (dd, J = 13.9, 11.4 Hz, 1H), 2.41-2.45 (m, 2H), 1.54-1.62 (m, 1H), 1.28-1.46 (m, 6H), 1.00 (d, J = 7.2 Hz, 3H), 0.76 (d, J = 6.1 Hz, 3H), 0.72 (d, J = 6.2 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.7, 172.7, 172.6, 172.5, 171.6, 158.9, 158.6, 141.9, 136.6, 132.6, 132.5, 130.4, 130.1, 128.9, 128.4, 126.9, 125.7, 124.3, 117.8, 115.4, 115.0, 68.2, 54.3, 52.6, 51.8, 48.8, 40.9, 36.8, 36.5, 30.9, 29.3, 25.3, 24.5, 23.4, 21.8, 18.5. MS (ESI) Calculated for C₃₆H₅₀N₈O₆[M+H]⁺: 691.4, found 691.3.

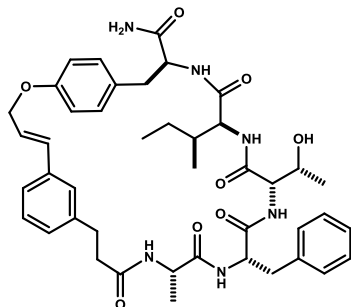
Cyclic-Ile-Met-Ser-Tyr-Trp (12):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (18 mg, 0.027mmol, 73%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.79 (s, 1H), 8.11 (d, J = 7.5 Hz, 1H), 7.97 (d, J = 8.1 Hz, 1H), 7.89 (d, J = 8.2 Hz, 1H), 7.81 (d, J = 7.5 Hz, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 7.2 Hz, 1H), 7.30 (d, J = 8.0 Hz, 1H), 7.17-7.24 (m, 4H), 7.11-7.16 (m, 4H), 7.01-7.08 (m, 2H), 6.97 (dd, J = 7.3, 7.3 Hz), 6.83 (d, J = 8.6 Hz, 2H), 6.56 (d, J = 15.9 Hz, 1H), 6.39 (dt, J = 16.1, 5.5 Hz, 1H), 4.76 (d, J = 5.2 Hz, 2H), 4.43 (ddd, J = 8.5, 8.5, 5.2 Hz, 1H), 4.22-4.33 (m, 3H), 4.10 (dd, J = 8.4, 6.0 Hz, 1H), 3.55 (dd, J = 10.4, 6.0 Hz, 1H), 3.49 (dd, J = 10.5, 6.7 Hz, 1H), 3.16 (dd, J = 14.7, 4.9 Hz, 1H), 2.82-2.96 (m, 3H), 2.70-2.77 (m, 1H), 2.50-2.60 (m, 2H), 2.40-2.46 (m, 1H), 2.27-2.39 (m, 1H), 1.92 (s,

3H), 1.71-1.89 (m, 2H), 1.60-1.69 (m, 1H), 1.12-1.20 (m, 1H), 0.85-0.95 (m, 1H), 0.56-0.62 (m, 6H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.8, 172.3, 171.49, 171.48, 171.3, 171.1, 157.1, 141.8, 136.7, 136.5, 132.7, 130.6, 130.2, 128.9, 128.6, 127.8, 126.2, 125.6, 124.7, 123.9, 121.3, 118.9, 118.8, 114.9, 111.7, 110.7, 68.1, 61.9, 57.7, 55.7, 55.2, 54.0, 52.2, 36.9, 36.4, 36.3, 32.0, 31.0, 29.6, 28.1, 24.5, 15.9, 14.9, 11.4. MS (ESI) Calculated for C₄₆H₅₇N₇O₈S [M+H]⁺: 868.4, found 868.0.

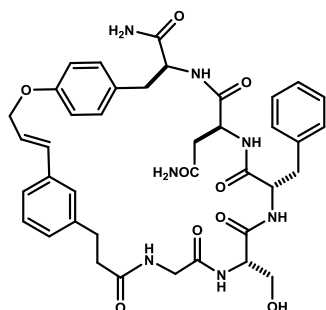
Cyclic-Ala-Phe-Thr-Ile-Tyr (13):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (14 mg, 0.018mmol, 85%). ¹H NMR (DMSO-d₆, 600 MHz): δ 8.10 (d, J = 7.3 Hz, 1H), 8.08 (d, J = 8.9 Hz, 1H), 7.55-7.62 (m, 4H), 7.49-7.54 (m, 3H), 7.30 (s, 1H), 7.23 (s, 1H), 7.15-7.20 (m, 6H), 7.09-7.14 (m, 3H), 7.01-7.05 (m, 2H), 6.79 (d, J = 8.5 Hz, 2H), 6.63 (d, J = 16.3 Hz, 1H), 6.40 (dt, J = 15.9, 5.7 Hz, 1H), 4.61-4.69 (m, 2H), 4.46 (ddd, J = 9.0, 9.0, 4.6 Hz, 1H), 4.34-4.39 (m, 1H), 4.20 (dd, J = 8.04, 4.6 Hz, 1H), 4.12-4.17 (m, 2H), 3.85 (dq, J = 5.7, 5.7 Hz, 1H), 3.04 (J = 14.0, 4.4 Hz, 1H), 2.85-2.90 (m, 1H), 2.69-2.84 (m, 4H), 2.29-2.36 (m,

1H), 1.62-1.70 (m, 1H), 1.28-1.36 (m, 1H), 1.04 (d, J = 7.0 Hz, 3H), 0.93-1.01 (m, 1H), 0.82 (d, J = 6.1 Hz, 3H), 0.76 (d, J = 6.6 Hz, 3H), 0.73 (t, J = 7.5 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.4, 172.8, 171.8, 171.1, 171.0, 169.5, 157.1, 141.8, 138.1, 136.4, 133.4, 132.7, 132.45, 132.37, 131.84, 131.77, 130.5, 130.1, 129.5, 129.1, 129.0, 128.7, 128.4, 128.3, 126.5, 125.7, 125.4, 124.6, 114.6, 68.2, 67.0, 58.1, 57.1, 54.2, 54.0, 48.7, 37.2, 37.0, 36.6, 35.7, 30.4, 24.3, 18.9, 18.5. MS (ESI) Calculated for C₄₃H₅₄N₆O₈ [M+H]⁺: 783.4, found 783.3.

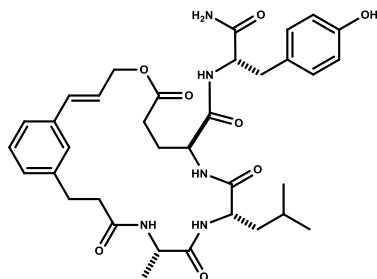
Cyclic-Gly-Ser-Phe-Asn-Tyr (14):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (12 mg, 0.016mmol, 74%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.17 (t, J = 5.7 Hz, 1H), 8.15 (d, J = 8.7 Hz, 1H), 8.06 (d, J = 7.9 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 8.1 Hz, 1H), 7.45 (br s, 1H), 7.28 (br s, 1H), 7.24 (d, J = 7.6 Hz, 1H), 7.17-7.22 (m, 2H), 7.12-7.17 (m, 3H), 7.05-7.11 (m, 3H), 7.04-7.10 (m, 5H), 6.95-7.01 (m, 1H), 6.80 (d, J = 8.9 Hz,

2H), 6.12 (d, J = 16.3 Hz, 1H), 6.33 (dt, J = 16.2, 5.8 Hz, 1H), 4.61 (d, J = 13.8, 6.2 Hz, 1H), 4.46-4.56 (m, 2H), 3.64 (ddd, J = 8.6, 8.6, 4.4 Hz), 4.30 (ddd, J = 7.6, 6.0, 6.0 Hz, 1H), 4.22 (ddd, J = 11.0, 8.2, 3.0 Hz, 1H), 3.77 (dd, J = 16.7, 6.0 Hz, 1H), 3.64 (dd, J = 16.6, 5.3 Hz, 1H), 3.42-3.50 (m, 2H), 3.07 (dd, J = 14.0, 3.0 Hz, 1H), 2.74-2.94 (m, 3H), 2.70 (dd, J = 14.0, 11.1 Hz, 1H), 2.49-2.61 (m, 3H), 2.38-2.46 (m, 1H), 2.35 (dd, J = 15.6, 6.0 Hz, 1H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.8, 172.43, 172.41, 171.0, 170.5, 170.1, 169.5, 157.2, 142.2, 137.8, 136.7, 132.9, 130.7, 130.5, 129.8, 128.8, 128.5, 128.4, 126.8, 126.6, 125.3, 124.2, 114.8, 68.5, 61.7, 55.2, 55.0, 54.1, 50.0, 42.6, 38.3, 37.5, 36.3, 36.1. MS (ESI) Calculated for C₃₉H₄₅N₇O₉ [M+H]⁺: 756.3, found 756.2.

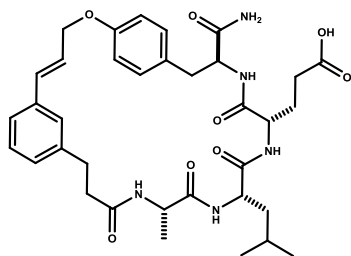
Cyclic-Ala-Leu-Glu-Tyr (16):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (17 mg, 0.026 mmol, 67%). ¹H NMR (DMSO-d₆, 600 MHz): δ 8.03 (d, J = 5.8 Hz, 1H), 7.99 (d, J = 7.2 Hz, 1H), 7.93 (d, J = 9.1 Hz, 1H), 7.45 (d, J = 7.9 Hz, 1H), 7.35-7.42 (m, 2H), 7.12-7.19 (m, 2H), 6.98-7.06 (m, 2H), 6.96 (d, J = 8.1 Hz, 2H), 6.59 (d, J = 8.2 Hz, 2H), 6.54 (d, J = 16.6 Hz, 1H), 6.33 (dt, J = 15.9, 4.6 Hz, 1H), 4.80-4.87 (m, 1H), 4.54-4.61 (m, 1H), 4.13-4.35 (m, 4H), 2.78-2.92 (m, 2H), 2.61-2.71 (m, 1H), 2.22-2.40 (m,

3H), 1.64-1.74 (m, 1H), 1.62-1.61 (m, 1H), 1.32-1.46 (m, 2H), 0.99 (d, J = 6.2 Hz, 3H), 0.85 (d, J = 6.2 Hz, 3H), 0.81 (d, J = 7.0 Hz, 3H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.1, 172.6, 172.4, 172.3, 171.6, 170.7, 156.1, 141.7, 136.4, 131.6, 130.4, 128.7, 128.4, 128.0, 125.5, 124.4, 123.9, 115.2, 63.4, 54.2, 51.6, 51.5, 48.4, 37.2, 34.1, 30.0, 29.9, 27.9, 24.5, 23.2, 22.1, 19.2. MS (ESI) Calculated for C₃₅H₄₅N₅O₈ [M+H]⁺: 664.3, found 664.2.

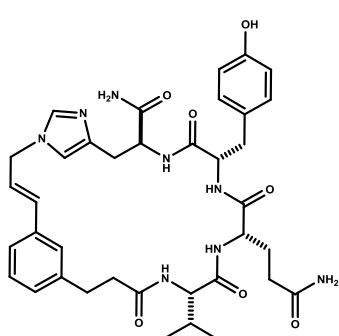
Cyclic-Ala-Leu-Glu-Tyr (17):



Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Xbridge RP18 20x250 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (11 mg, 0.160 mmol, 76%). ¹H NMR (DMSO-d₆, 600 MHz): δ 12.04 (s, 1H), 8.1 (d, J = 6.9 Hz, 1H), 7.82 (d, J = 7.8 Hz, 1H), 7.71 (d, J = 8 Hz, 1H), 7.56 (d, J = 7.2 Hz, 1H), 7.31 (br. s, J = Hz, 1H), 7.17-7.22 (m, 3H), 7.02-7.13 (m, 4H), 6.83 (d, J = 8.6 Hz, 2H), 6.65 (d, J = 16 Hz, 1H), 6.37 (dt, J = 16.0, 5.6 Hz, 1H), 4.76 (d, J = 5.1 Hz, 2H), 4.32 (ddd, J = 10.9, 8.1, 3.1 Hz, 1H), 4.18 (dt, J = 7.6, 7.6 Hz, 1H), 4.02-4.13 (m, 2H), 2.96 (ddd, J =

14.2, 2.8 Hz, 1H), 2.76-2.82 (m, 2H), 2.67 (ddd, J = 14.3, 10.9 Hz, 1H), 2.36-2.42 (m, 1H), 2.11-2.23 (m, 2H), 1.79-1.89 (m, 1H), 1.66-1.76 (m, 1H), 1.57 (dddd, J = 13.3, 13.3, 6.7, 6.7 Hz, 1H), 1.40-1.48 (m, 2H), 1.03 (d, J = 7.2 Hz, 3H), 0.84 (d, J = 6.6 Hz, 3H), 0.81 (d, J = 6.6 Hz, 3H). ¹³C NMR (DMSO-d₆, 150 MHz): δ 173.9, 172.6, 172.2, 171.85, 171.8, 170.9, 156.6, 141.4, 136.0, 132.4, 132.3, 130.2, 128.3, 127.9, 126.0, 125.4, 124.3, 114.5, 67.7, 54.0, 51.6, 51.1, 48.9, 40.1, 36.3, 35.6, 30.2, 29.6, 26.7, 23.5, 22.9, 21.2, 17.3. MS (ESI) Calculated for C₃₅H₄₅N₅O₈ [M+H]⁺: 664.3, found 664.3.

Cyclic-Val-Gln-Tyr-His (19):

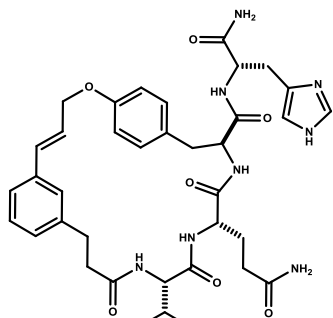


Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (14mg, 0.020 mmol, 75%). ¹H NMR (DMSO-d₆, 500 MHz): δ 9.16 (br. s, J = Hz, 1H), 9.02 (s, 1H), 8.31 (br. s, J = Hz, 1H), 8.1 (d, J = 8.3 Hz, 1H), 7.93 (d, J = 6.9 Hz, 1H), 7.73 (d, J = 5.6 Hz, 1H), 7.26-7.36 (m, 4H), 7.21 (d, J = 7.5 Hz, 1H), 7.15 (br. d, J = 7.8 Hz, 1H), 7.11 (br. d, J = 7.5 Hz, 1H), 7.01 (br. s, J = Hz, 1H), 6.97 (d, J = 8.6 Hz, 2H), 6.81 (br. s, J = Hz, 1H), 6.75 (d, J = 15.6 Hz, 1H), 6.59 (d, J = 8.4 Hz, 2H), 6.38 (dt, J = 15.4, 7.0 Hz, 1H), 4.92 (dd, J = 14.9, 5.9 Hz, 1H), 4.88 (dd, J = 14.9, 7.3 Hz, 1H), 4.47 (ddd, J = 10.6, 8.5, 3.4 Hz, 1H), 4.28 (ddd, J = 8.9, 7.9, 5.0 Hz, 1H), 3.99 (ddd, J = 7.8, 5.7, 5.7 Hz, 1H), 3.82-3.88 (m, 1H), 3.16 (dd,

J = 15.2, 3.1 Hz, 1H), 2.86-2.94 (m, 2H), 2.79-2.85 (m, 2H), 2.74 (dd, J = 14.3, 9.4 Hz, 1H), 2.54-2.63 (m, 1H), 2.45-2.5 (m, 1H), 1.98-

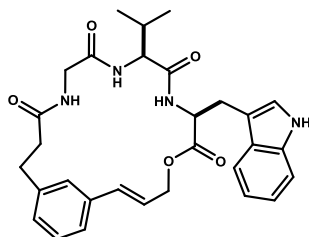
2.13 (m, 2H), 1.92 (ddd, J = 13.6, 12.5, 6.8 Hz, 1H), 1.77 (ddd, J = 13.8, 13.8, 7.0 Hz, 1H), 1.65 (ddd, J = 14.6, 14.6, 7.6 Hz, 1H), 0.67 (dd, J = 6.7, 2.0 Hz, 6H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 174.0, 173.1, 173.0, 172.2, 172.1, 171.1, 155.7, 141.4, 135.7, 135.5, 134.8, 134.3, 130.7, 130.1, 129.0, 128.4, 125.6, 125.5, 122.2, 118.2, 114.9, 59.0, 54.7, 53.9, 51.1, 50.1, 35.9, 35.6, 31.1, 30.6, 29.0, 26.6, 26.4, 18.2. MS (ESI) Calculated for C₃₇H₄₆N₈O₇ [M+H]⁺: 715.4, found 715.0

Cyclic-Val-Gln-Tyr-His (20):



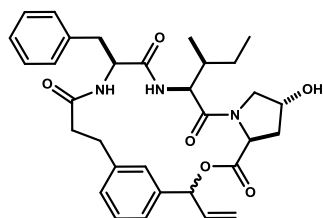
Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (12 mg, 0.017 mmol, 68%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.95 (d, J = 1.1 Hz, 1H), 8.28 (d, J = 8.3 Hz, 1H), 7.92 (d, J = 6.9 Hz, 1H), 7.85 (d, J = 7.6 Hz, 1H), 7.50-7.55 (m, 2H), 7.34-7.38 (m, 2H), 7.28 (br. s, J = Hz, 2H), 7.14-7.17 (m, 2H), 7.13 (d, J = 8.7 Hz, 2H), 7.00-7.04 (m, 1H), 6.84 (d, J = 8.7 Hz, 2H), 6.81 (br. s, J = Hz, 1H), 6.67 (d, J = 16 Hz, 1H), 6.55 (ddd, J = 15.9, 6.6, 5.6 Hz, 1H), 4.78 (dd, J = 14.5, 4.9 Hz, 1H), 4.7 (dd, J = 14.5, 6.9 Hz, 1H), 4.52 (ddd, J = 8.2, 8.2, 5.5 Hz, 1H), 4.26 (ddd, J = 10.0, 7.0, 2.4 Hz, 1H), 4.15 (ddd, J = 7.5, 7.5, 7.5 Hz, 1H), 3.94 (dd, J = 8.6, 6.7 Hz, 1H), 3.11 (dd, J = 15.5, 5.4 Hz, 1H), 2.92 (dd, J = 15.3, 8.2 Hz, 1H), 2.80-2.88 (m, 3H), 2.65 (dd, J = 14.1, 11.7 Hz, 1H), 2.33-2.42 (m, 1H), 1.96-2.09 (m, 2H), 1.71-1.80 (m, 1H), 1.55-1.64 (m, 1H), 1.42 (ddd, J = 13.4, 13.4, 6.7 Hz, 1H), 0.21 (d, J = 7.1 Hz, 3H), 0.19 (d, J = 7.8 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 174.5, 172.2, 171.9, 171.5, 171.0, 157.2, 141.0, 136.7, 134.14, 134.07, 130.6, 129.9, 129.6, 129.2, 128.7, 125.7, 125.4, 125.2, 117.3, 114.9, 68.4, 57.2, 55.5, 52.0, 51.8, 36.3, 34.4, 32.2, 31.8, 30.6, 27.4, 26.9, 19.1, 18.2. MS (ESI) Calculated for C₃₇H₄₆N₈O₇ [M+H]⁺: 715.4, found 715.4

Cyclic-Gly-Val-Trp (21):

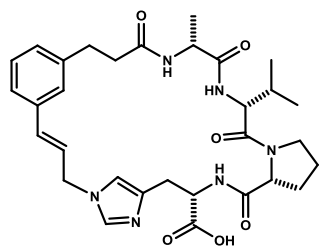


Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (21 mg, 0.039 mmol, 74%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.82 (s, 1H), 8.31 (d, J = 7.2 Hz, 1H), 8.18 (dd, J = 6.8, 4.3 Hz, 1H), 7.55 (d, J = 8.3 Hz, 1H), 7.47 (d, J = 8.3 Hz, 1H), 7.27-7.31 (m, 2H), 8.10-7.18 (m, 3H), 7.00-7.05 (m, 2H), 6.95 (dd, J = 7.8, 7.8 Hz, 1H), 6.58 (d, J = 15.9 Hz, 1H), 6.11 (dt, J = 16.0, 5.3 Hz, 1H), 4.79 (ddd, J = 13.9, 5.0, 1.3 Hz, 1H), 4.40-4.48 (m, 2H), 4.02-4.48 (m, 2H), 4.02-4.14 (m, 3H), 3.57 (dd, J = 17.3, 3.9 Hz, 1H), 3.20 (dd, J = 14.8, 5.9 Hz, 1H), 3.10 (dd, J = 14.9, 9.1 Hz, 1H), 2.91-2.97 (m, 1H), 2.82 (ddd, J = 14.7, 8.9, 1.9 Hz, 1H), 2.59 (ddd, J = 15.2, 9.8, 2.1 Hz, 1H), 2.32 (ddd, J = 15.2, 8.9, 2.5 Hz, 1H), 1.90-1.98 (m, 1H), 0.69 (d, J = 6.8 Hz, 3H), 0.60 (d, J = 7.0 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 172.3, 171.6, 171.0, 169.4, 141.9, 136.5, 136.4, 131.4, 128.3, 128.2, 127.3, 125.4, 123.9, 123.5, 123.2, 120.9, 118.4, 117.9, 111.3, 110.0, 64.4, 57.1, 53.4, 42.2, 35.4, 30.6, 29.6, 26.3, 19.3, 17.0. MS (ESI) Calculated for C₃₀H₃₄N₄O₅ [M+H]⁺: 531.3, found 531.3.

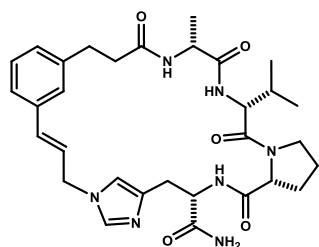
Cyclic-Phe-Leu-Hyp (22):



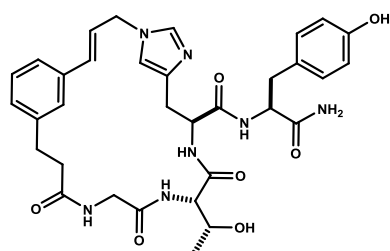
Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (16 mg, 0.029 mmol, 71%). ¹H NMR (DMSO-d₆, 500 MHz, mix of diastereomers): δ 8.35 (d, J = 7.6 Hz, 1H), 8.28 (d, J = 8.3 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 7.32-7.37 (m, 3H), 7.12-7.29 (m, 1H), 6.98-7.10 (m, 4H), 6.83 (ddd, J = 16.0, 9.0, 4.1 Hz, 1H), 6.65 (d, J = 16.2 Hz, 1H), 6.59 (d, J = 16.2 Hz, 1H), 6.12 (ddd, J = 16.2, 6.0, 4.0 Hz, 1H), 5.28 (ddd, J = 12.5, 3.9, 1.7 Hz, 1H), 5.02 (ddd, J = 14.1, 3.8, 1.7 Hz, 1H), 4.32-4.57 (m, 10H), 3.94-3.60 (m, 4H), 3.13 (dd, J = 14.2, 4.5 Hz, 2H), 2.94-3.07 (m, 3H), 2.64-2.73 (m, 3H), 2.50-2.58 (m, 2H), 2.38-2.46 (m, 2H), 2.24-2.34 (m, 2H), 2.07-2.21 (m, 2H), 1.88 (ddd, J = 13.7, 10.2, 4.1 Hz, 1H), 1.62-1.72 (m, 1H), 1.53 (ddd, J = 14.3, 12.4, 3.4 Hz, 1H), 1.32-1.43 (m, 1H), 1.18-1.29 (m, 3H), 1.06 (ddd, J = 14.2, 10.9, 3.4 Hz, 1H), 0.85 (d, J = 6.7 Hz, 3H), 0.83 (d, J = 6.4 Hz, 3H), 0.74 (d, J = 6.4 Hz, 3H), 0.53 (d, J = 6.6 Hz, 3H). MS (ESI) Calculated for C₃₂H₃₉N₃O₈ [M+H]⁺: 562.3, found 562.3.

Cyclic-Ala-Val-Pro-His-OH (23):

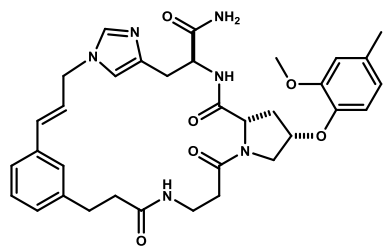
Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (16 mg, 0.029mmol, 69%). ¹H NMR (DMSO-d₆, 500 MHz): δ 9.05 (s, 1H), 8.12 (d, J = 7.9 Hz, 1H), 8.04 (d, J = 7.7 Hz, 1H), 7.48 (s, 1H), 7.43 (d, J = 8.9 Hz, 1H), 7.16-7.27 (m, 3H), 7.09-7.14 (m, 1H), 6.66 (d, J = 15.9 Hz, 1H), 6.34 (dt, J = 16.0, 6.6 Hz, 1H), 4.84-4.98 (m, 2H), 4.22-4.30 (m, 2H), 4.18 (dd, J = 8.5, 3.6 Hz, 1H), 4.09 (t, J = 8.9 Hz, 1H), 3.55-3.63 (m, 1H), 3.48-3.46 (m, 1H), 3.05-3.18 (m, 2H), 2.9 (ddd, J = 14.7, 9.9, 4.3 Hz, 1H), 2.7 (ddd, J = 11.2, 6.4, 4.4 Hz, 1H), 2.61 (ddd, J = 15.0, 10.2, 4.1 Hz, 1H), 2.33-2.41 (m, 1H), 1.60-1.86 (m, 3H), 1.13 (d, J = 7.1 Hz, 3H), 0.79 (d, J = 6.6 Hz, 3H), 0.57 (d, J = 6.7 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 172.5, 172.13, 172.07, 171.5, 170.5, 141.9, 135.9, 135.4, 135.0, 130.9, 129.0, 129.0, 127.1, 124.2, 122.6, 120.4, 60.0, 56.0, 51.4, 50.9, 48.6, 47.4, 35.3, 30.6, 29.9, 29.5, 26.0, 24.6, 19.5, 18.6, 18.5. MS (ESI) Calculated for C₃₁H₄₀N₆O₆ [M+H]⁺: 593.3, found 593.1

Cyclic-Ala-Val-Pro-His-NH₂ (24):

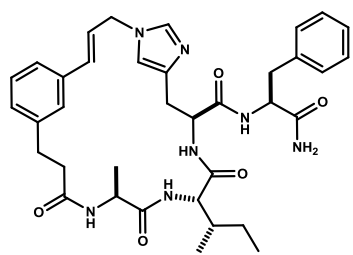
Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (74 mg, 0.13mmol, 77%). ¹H NMR (DMSO-d₆, 500 MHz): δ 9.08 (d, J = 1.4 Hz, 1H), 8.17 (d, J = 8.3 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 8.9 Hz, 1H), 7.40 (s, 1H), 7.34 (br. s, 1H), 7.21-7.29 (m, 2H), 7.11-7.20 (m, 3H), 6.56 (d, J = 16.0 Hz, 1H), 6.35 (dt, J = 16.0, 6.2 Hz, 1H), 4.89-5.00 (m, 2H), 4.25-4.36 (m, 2H), 4.11-4.19 (m, 2H), 3.53-3.61 (m, 1H), 3.29-3.37 (m, 1H), 3.03-3.13 (m, 2H), 2.79-2.89 (m, 1H), 2.65-2.73 (m, 1H), 2.48-2.55 (m, 1H), 2.40 (ddd, J = 15.0, 6.5, 6.5 Hz, 1H), 1.79-1.88 (m, 1H), 1.63-1.77 (n, 2H), 1.52-1.62 (m, 1H), 1.12 (d, J = 7.0 Hz, 3H), 0.75 (d, J = 6.7 Hz, 3H), 0.71 (d, J = 6.6 Hz, 1H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 172.6, 172.2, 172.1, 171.6, 170.7, 142.1, 135.9, 135.1, 134.5, 130.7, 129.0, 128.5, 127.8, 124.1, 123.3, 120.4, 60.4, 56.1, 51.9, 50.6, 49.1, 48.2, 47.5, 35.7, 30.8, 29.9, 29.3, 26.4, 24.9, 19.6, 18.6, 18.0. MS (ESI) Calculated for C₃₁H₄₁N₇O₅ [M+H]⁺: 592.3, found 592.3

Cyclic-Gly-Thr-His-Tyr-NH₂ (25):

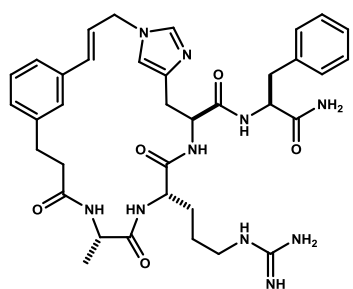
Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Xbridge RP18 20x250 mm) using a gradient of 25-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (24 mg, 0.038mmol, 73%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.99 (br. s, 1H), 8.14 (t, J = 5.9 Hz, 2H), 8.05 (d, J = 8.3 Hz, 1H), 7.96 (d, J = 7.7 Hz, 1H), 7.73 (d, J = 8.2 Hz, 1H), 7.54 (br. s, 1H), 7.4 (br. s, 1H), 7.36 (br. s, 1H), 7.19-7.22 (m, 2H), 7.16 (br. d, J = 7.6 Hz, 1H), 7.08 (br. d, J = 7.6 Hz, 1H), 7 (d, J = 8.5 Hz, 2H), 6.74 (d, J = 15.7 Hz, 1H), 6.61 (d, J = 8.1 Hz, 2H), 6.49 (dt, J = 15.6, 7.1 Hz, 1H), 4.92 (dd, J = 14.8, 6.4 Hz, 1H), 4.8 (dd, J = 14.8, 7.3 Hz, 1H), 4.53 (ddd, J = 8.5, 8.5, 3.8 Hz, 1H), 4.28 (ddd, J = 8.7, 8.7, 4.7 Hz, 1H), 4.63 (dd, J = 7.6, 4.0 Hz, 1H), 3.92 (dq, J = 6.2, 6.2 Hz, 1H), 3.8 (dd, J = 15.6, 5.6 Hz, 1H), 3.75 (dd, J = 16.6, 6.2 Hz, 1H), 3.05 (dd, J = 15.5, 3.6 Hz, 1H), 2.81-2.94 (m, 4H), 2.67 (dd, J = 13.8, 9.3 Hz, 1H), 2.34-2.41 (m, 1H), 1.04 (d, J = 6.4 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.7, 172.2, 170.5, 170.1, 169.9, 156.3, 142.3, 136.8, 136.0, 134.7, 130.6, 130.2, 129.5, 128.8, 128.2, 125.6, 125.4, 122.3, 120.2, 115.4, 67.2, 58.6, 55.1, 51.5, 51.0, 42.0, 37.1, 35.4, 29.9, 26.9, 20.2. MS (ESI) Calculated for C₃₃H₃₉N₇O₇ [M+H]⁺: 646.3, found 646.1.

Cyclic-β-Ala-Pro[4-(2-methoxy-4-methylphenoxy)]-His (26):

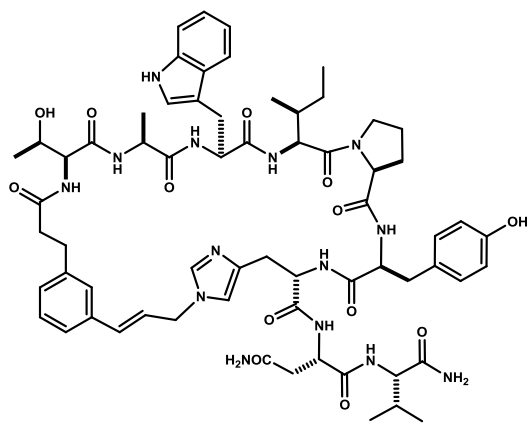
Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (57 mg, 0.091 mmol, 81%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.85 (d, J = 1.2 Hz, 1H), 7.78 (d, J = 7.5 Hz, 1H), 7.65 (t, J = 5.7 Hz, 1H), 7.21-7.31 (m, 5H), 7.15-7.20 (m, 2H), 6.83 (d, J = 8 Hz, 1H), 6.78 (d, J = Hz, 1H), 6.66-6.74 (m, 2H), 6.38 (dt, J = 15.7, 7.0 Hz, 1H), 4.89 (dd, J = 14.8, 6.4 Hz, 1H), 4.70-4.75 (m, 1H), 4.59 (dd, J = 14.7, 7.3 Hz, 1H), 4.35-4.42 (m, 2H), 3.71 (s, 3H), 3.67-3.70 (m, 1H), 3.34 (br. d, J = 11.3 Hz, 1H), 3.17 (m, 1H), 3.07 (d, J = 6.4 Hz, 2H), 2.92-3.00 (m, 1H), 2.84-2.90 (m, 1H), 2.78-2.83 (m, 1H), 2.27-2.41 (m, 3H), 2.25 (s, 3H), 2.15-2.23 (m, 2H), 1.85-2.00 (m, 2H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 171.5, 171.2, 171.0, 170.6, 150.1, 143.4, 142.6, 141.3, 136.1, 134.6, 132.5, 132.2, 129.1, 128.5, 126.7, 124.9, 122.2, 120.8, 118.8, 118.1, 113.4, 77.9, 58.7, 55.4, 52.7, 50.9, 50.3, 36.7, 34.4, 33.8, 33.5, 31.4, 20.7. MS (ESI) Calculated for C₃₄H₄₀N₆O₆ [M+H]⁺: 629.3, found 629.3

Cyclic-Ala-Ile-His-Phe-NH₂ (27):

Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (25 mg, 0.032 mmol, 71%). ¹H NMR (DMSO-d₆, 500 MHz): δ 9.04 (d, J = 1.5 Hz, 1H), 8.12 (d, J = 8.6 Hz, 1H), 8 (d, J = 5.7 Hz, 1H), 7.86 (d, J = 8.1 Hz, 1H), 7.75 (d, J = 7.3 Hz, 1H), 7.59 (br. s, 1H), 7.55 (br. s, 1H), 7.44 (br. s, 1H), 7.14-7.25 (m, 7H), 7.1 (d, J = 7.7 Hz, 1H), 7.06 (d, J = 7.7 Hz, 1H), 6.71-6.82 (m, 2H), 4.85-4.96 (m, 2H), 4.61 (ddd, J = 8.3, 9.3, 3.8 Hz, 1H), 4.44 (ddd, J = 8.1, 8.1, 5.0 Hz, 1H), 4.14 (dq, J = 6.7, 6.7 Hz, 1H), 3.86 (t, J = 7.6 Hz, 1H), 2.87-3.04 (m, 4H), 2.81 (ddd, J = 13.8, 8.3 Hz, 1H), 2.70-2.77 (m, 1H), 2.40-2.46 (m, 2H), 1.52-1.62 (m, 1H), 1.36-1.46 (m, 1H), 1 (d, J = 7 Hz, 3H), 0.74 (t, J = 7.5 Hz, 3H), 0.75 (d, J = 6.8 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.2, 173.1, 172.0, 171.8, 170.2, 142.1, 137.8, 136.2, 136.1, 134.8, 130.5, 129.7, 129.5, 128.7, 128.5, 126.8, 126.1, 124.6, 123.1, 119.8, 57.9, 54.2, 51.2, 51.1, 48.8, 38.2, 36.1, 34.5, 29.9, 27.3, 25.1, 18.4, 15.8, 11.4. MS (ESI) Calculated for C₃₆H₄₅N₇O₅ [M+H]⁺: 656.3, found 656.2

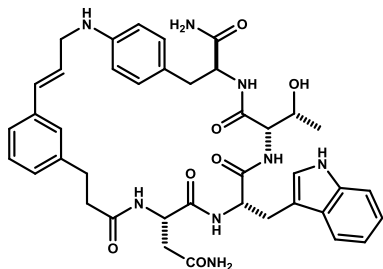
Cyclic-Ala-Arg-His-Phe-NH₂ (28):

Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (36 mg, 0.044mmol, 76%). ¹H NMR (DMSO-d₆, 500 MHz): δ 9.03 (s, 1H), 8.11-8.14 (m, 2H), 7.97 (d, J = 6.2 Hz, 1H), 7.96 (d, J = 7.7 Hz, 1H), 7.7 (br. s, 1H), 7.48 (br. s, 1H), 7.38-7.41 (m, 2H), 7.28 (br. s, 1H), 7.14-7.25 (m, 7H), 7.1 (d, J = 7.4 Hz, 1H), 7.04 (d, J = 7.6 Hz, 1H), 6.8 (ddd, J = 15.7, 7.9, 5.6 Hz, 1H), 6.74 (d, J = 15.7 Hz, 1H), 4.91 (dd, J = 14.6, 5.2 Hz, 1H), 4.86 (dd, J = 14.8, 8.0 Hz, 1H), 4.57 (ddd, J = 8.7, 8.7, 3.5 Hz, 1H), 4.41 (ddd, J = 8.5, 8.5, 4.9 Hz, 1H), 4.05 (dq, J = 7.2, 7.2 Hz, 1H), 3.91-3.96 (m, 1H), 2.96-3.03 (m, 5H), 2.88 (dd, J = 15.6, 9.4 Hz, 1H), 2.79 (dd, J = 13.8, 8.9 Hz, 1H), 2.71 (dd, J = 15.0, 7.8 Hz, 1H), 2.34-2.41 (m, 2H), 1.40-1.52 (m, 4H), 1.09 (d, J = 7 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.5, 173.4, 172.3, 172.1, 170.2, 157.1, 142.1, 137.9, 136.3, 136.3, 134.8, 130.4, 129.7, 129.4, 128.7, 128.6, 126.9, 126.1, 124.5, 123.0, 119.7, 117.6, 115.3, 54.3, 52.9, 51.1, 51.0, 49.0, 40.9, 38.1, 34.4, 29.7, 28.7, 27.5, 25.6, 18.1. MS (ESI) Calculated for C₃₆H₄₆N₁₀O₅ [M+H]⁺: 699.4, found 699.2

Cyclic-Thr-Ala-Trp-Ile-Pro-Tyr-His-Asn-Val (29):

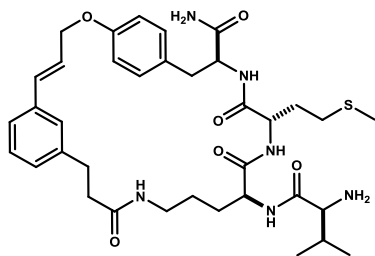
Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (25 mg, 0.020 mmol, 69%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.8 (d, J = 1.7 Hz, 1H), 9.04 (s, 1H), 8.33 (d, J = 7.2 Hz, 1H), 8.18 (d, J = 7.3 Hz, 1H), 7.98 (d, J = 6 Hz, 1H), 7.89 (d, J = 7.8 Hz, 1H), 7.73-7.82 (m, 2H), 7.54 (d, J = 8.7 Hz, 1H), 7.40-7.48 (m, 3H), 7.28-7.32 (m, 2H), 7.12-7.21 (m, 6H), 7.08-7.11 (m, 2H), 7.00-7.05 (m, 3H), 6.94 (t, J = 7.3 Hz, 1H), 6.63 (d, J = 15.9 Hz, 1H), 6.44 (dt, J = 15.9, 6.5 Hz, 1H), 4.9 (d, J = 6.1 Hz, 2H), 4.53-4.61 (m, 2H), 4.25-4.40 (m, 4H), 4.06-4.16 (m, 3H), 3.99 (dq, J = 6.9, 6.9 Hz, 1H), 3.37-3.44 (m, 1H), 3.14 (ddd, J = 15.6, 15.6, 4.8 Hz, 1H), 2.89-3.03 (m, 2H), 2.63-2.66 (m, 3H), 2.50-2.60 (m, 2H), 2.28-2.31 (m,

1H), 2.02 (dddd, J = 13.3, 6.7, 6.7, 6.7 Hz, 1H), 1.84-1.92 (m, 1H), 1.58-1.75 (m, 3H), 1.37-1.47 (m, 1H), 1.04 (d, J = 7.2 Hz, 3H), 0.94-1.01 (m, 1H), 0.93 (d, J = 6 Hz, 3H), 0.8 (d, J = 7.3 Hz, 3H), 0.79 (d, J = 6.7 Hz, 3H), 0.7 (d, J = 7.3 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.1, 172.7, 172.4, 172.4, 172.1, 171.7, 171.5, 171.3, 170.7, 170.2, 170.1, 142.2, 138.4, 136.5, 136.0, 135.1, 135.0, 130.1, 129.4, 128.9, 128.5, 127.7, 126.75, 126.70, 125.1, 123.9, 123.0, 121.3, 120.3, 118.8, 118.6, 117.7, 115.4, 111.8, 110.5, 67.1, 60.3, 58.5, 58.0, 55.5, 54.9, 54.6, 51.7, 50.7, 50.5, 49.8, 47.5, 37.5, 37.1, 36.8, 36.5, 31.8, 30.7, 29.4, 27.6, 27.4, 24.6, 24.5, 20.2, 19.8, 18.0, 17.9, 15.7, 11.3. MS (ESI) Calculated for C₆₅H₈₄N₁₄O₁₃ [M+H]⁺: 1269.6, found 1269.4

Cyclic-Asn-Trp-Thr-Phe(4-NH₂) (30):

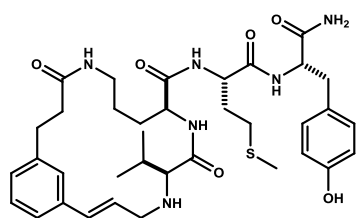
Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Xbridge RP18 20x250 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (48 mg, 0.064 mmol, 77%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.81 (d, J = 1.4 Hz, 1H), 8.31 (d, J = 6.1 Hz, 1H), 7.9 (d, J = 5.8 Hz, 1H), 7.55 (d, J = 7.3 Hz, 1H), 7.45-7.52 (m, 1H), 7.28 (d, J = 8.1 Hz, 1H), 7.19-7.25 (m, 4H), 7.17 (d, J = 7.5 Hz, 1H), 7.08-7.14 (m, 2H), 6.99-7.08 (m, 4H), 6.89-6.96 (m, 1H), 6.51 (d, J = 15.9 Hz, 1H), 6 (dt, J = 15.7, 6.5 Hz, 1H), 4.41 (ddd, J = 6.6, 6.6, 6.6 Hz, 1H), 4.33 (ddd, J = 5.9, 5.9, 5.9

Hz, 1H), 4.26 (ddd, J = 10.9, 7.9, 3.0 Hz, 1H), 3.89-3.98 (m, 2H), 3.81-3.88 (m, 2H), 3.03-3.11 (m, 3H), 2.63-2.80 (m, 3H), 2.26-2.45 (m, 4H), 0.7 (d, J = 6.1 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.8, 173.1, 172.6, 172.4, 172.0, 170.5, 142.1, 136.6, 136.3, 130.5, 129.1, 128.5, 127.8, 126.4, 125.0, 124.5, 121.4, 119.4, 118.8, 118.7, 118.5, 117.1, 114.8, 112.5, 111.8, 109.7, 66.6, 59.9, 55.2, 54.8, 51.4, 36.8, 36.7, 36.4, 30.6, 27.1, 19.4. MS (ESI) Calculated for C₄₀H₄₆N₈O₇ [M+H]⁺: 751.4, found 751.2.

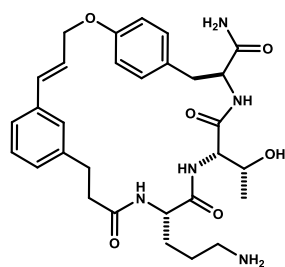
Cyclic-Val-Orn-Met-Try (32):

Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters Xbridge RP18 20x250 mm) using a gradient of 20-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (12 mg, 0.017 mmol, 64%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.38 (d, J = 7.9 Hz, 1H), 8.11 (d, J = 8.3 Hz, 1H), 7.97-8.04 (m, 4H), 7.72 (dd, J = 5.2, 5.2 Hz, 1H), 7.55 (s, 1H), 7.31 (s, 1H), 7.15-7.20 (m, 3H), 7.13 (br. d, J = 7.6 Hz, 1H), 7.06 (br. s, J = Hz, 1H), 7.01 (br. d, J = 7.4 Hz, 1H), 6.83 (br. d, J = 8.1 Hz, 2H), 6.67 (d, J = 15.9 Hz, 1H), 6.31 (dt, J = 15.9, 6.0 Hz, 1H), 4.73-4.81 (m, 2H), 4.29-4.38 (m, 2H), 4.21-4.27 (m, 1H), 3.52-

3.58 (m, 1H), 2.95-3.02 (m, 1H), 2.84-2.94 (m, 2H), 2.71-2.72 (m, 2H), 2.62 (dd, J = 12.9, 12.2 Hz, 1H), 2.31-2.37 (m, 2H), 2.21-2.22 (n, J = Hz, 1H), 1.93-2.01 (n, J = Hz, 4H), 1.86-1.93 (n, J = Hz, 1H), 1.71 (ddd, J = 15.1, 15.1, 7.7 Hz, 1H), 1.42-1.50 (m, 1H), 1.31-1.40 (m, 2H), 1.20-1.28 (m, 1H), 0.88 (d, J = 7 Hz, 6H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.6, 171.8, 171.32, 171.28, 168.1, 157.0, 142.1, 136.5, 133.0, 130.8, 130.7, 129.0, 128.7, 125.8, 125.7, 125.4, 114.8, 67.7, 57.6, 55.3, 52.6, 52.0, 38.5, 37.9, 37.2, 33.6, 31.8, 30.4, 29.5, 25.8, 18.7, 18.2, 15.0. MS (ESI) Calculated for C₃₆H₅₀N₆O₆S [M+H]⁺: 695.4, found 695.2

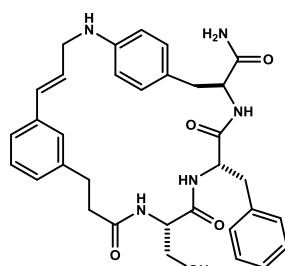
Cyclic-Val-Orn-Met-Try (33):

Following general procedure C, the corresponding compound was isolated by preparative HPLC (Waters XbridgeRP18 20x250 mm) using a gradient of 25-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (12 mg, 0.017mmol, 77%). ¹H NMR (DMSO-d₆, 500 MHz): δ 8.91 (br. s, J = Hz, 2H), 8.48 (d, J = 7 Hz, 1H), 8.09 (d, J = 8.2 Hz, 1H), 7.74 (dd, J = 6.6, 5.3 Hz, 1H), 7.68 (d, J = 8.1 Hz, 1H), 7.35-7.39 (m, 2H), 7.27 (t, J = 7.9 Hz, 1H), 7.15 (br. d, J = 7.9 Hz, 1H), 7.02 (br. s, J = Hz, 1H), 6.93-6.97 (m, 3H), 6.59 (d, J = 8.6 Hz, 2H), 6.52 (br. d, J = 15.7 Hz, 1H), 6.05 (dt, J = 15.4, 7.7 Hz, 1H), 4.3 (ddd, J = 8.3, 8.3, 5.3 Hz, 1H), 4.25 (ddd, J = 8.8, 8.8, 4.6 Hz, 1H), 4.01-4.07 (m, 1H), 3.71-3.79 (m, 1H), 3.52-3.64 (m, 2H), 3 (ddd, J = 14.7, 14.7, 7.7 Hz, 1H), 2.75-2.89 (m, 4H), 2.65 (dd, J = 13.8, 8.6 Hz, 1H), 2.40-2.47 (m, 1H), 2.35-2.39 (m, 1H), 2.25-2.34 (m, 2H), 2.04 (ddd, J = 13.8, 12.2, 6.9 Hz, 1H), 1.98 (s, 3H), 1.79-1.87 (m, 1H), 1.63-1.72 (m, 1H), 1.30-1.39 (m, 1H), 1.10-1.25 (m, 3H), 0.95 (d, J = 6.9 Hz, 3H), 0.91 (d, J = 6.7 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 172.6, 171.1, 170.6, 170.4, 166.0, 155.9, 141.1, 138.5, 134.5, 130.2, 129.3, 129.0, 128.4, 127.6, 122.0, 117.3, 114.8, 62.0, 53.9, 53.5, 51.6, 48.6, 36.6, 36.0, 34.8, 32.0, 30.6, 30.0, 29.1, 28.4, 27.0, 18.2, 17.9. MS (ESI) Calculated for C₃₆H₅₀N₆O₆S [M+H]⁺: 695.4, found 695.4

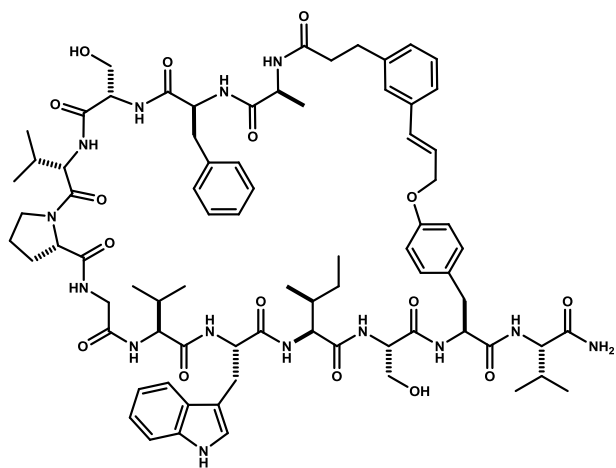
Cyclic-Orn-Thr-Try (35):

Following general procedure D, the corresponding compound was isolated by preparative HPLC (Waters Xbridge RP18 20x250 mm) using a gradient of 10-70% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (22 mg, 0.033mmol, 80%). ¹H NMR (DMSO-d₆, 600 MHz): δ 7.90 (d, J = 8.3 Hz, 1H), 7.90 (d, J = 8.3 Hz, 1H), 7.64 (d, J = 7.8 Hz, 1H), 7.53 (br s, 3H), 7.37 (s, 1H), 7.20-7.22 (m, 2H), 7.41 (br s, 1H), 7.19 (br s, 1H), 7.13 (d, J = 8.6 Hz, 2H), 7.04-7.08 (m, 1H), 6.85 (d, J = 8.6 Hz, 2H), 6.66 (d, J = 15.9 Hz, 1H), 6.46 (dt, J = 15.9, 5.8 Hz, 1H), 4.78 (d, J = 5.8 Hz, 2H), 4.34 (ddd, J = 10.6, 8.3, 2.8 Hz, 1H), 4.21 (ddd, J = 8.3, 8.1, 5.3 Hz, 1H), 4.14 (dd, J = 7.8, 5.2 Hz, 1H), 3.94 (tdd, J = 6.3, 5.9, 5.2 Hz, 1H), 2.88 (ddd, J = 14.7, 6.8, 4.5 Hz, 1H), 2.82 (ddd, J = 14.7, 10.1, 4.1 Hz, 1H), 3.00 (dd, J = 14.2, 2.8 Hz, 1H), 2.74 (dd, J = 14.2, 10.6 Hz, 1H), 2.69 (14.5, 10.1, 4.5 Hz, 1H), 2.48-2.55 (m, 2H), 2.37 (ddd, J = 14.5, 6.8, 4.1 Hz, 1H), 1.31-1.39 (m, 1H), 1.06-1.20 (m, 3H), 1.01 (d, J = 6.3 Hz, 3H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 172.9, 171.1, 170.7, 169.3, 156.4, 140.9, 135.8, 132.8, 129.9, 129.6, 128.4, 128.2, 125.0, 124.9, 124.2, 114.4, 67.7, 65.6, 57.8, 53.8, 51.0, 37.8, 35.7, 34.4, 29.9, 29.4, 22.5, 19.1.

MS (ESI) Calculated for C₃₀H₃₉N₅O₆ [M+H]⁺: 566.3, found 566.2.

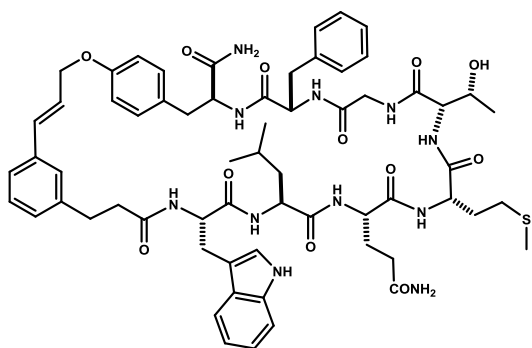
Cyclic-Ser-Phe-Phe(4-NH₂) (37):

Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (13 mg, 0.023 mmol, 72%). ¹H NMR (DMSO-d₆, 500 MHz): δ 7.99 (d, J = 8.7 Hz, 1H), 7.77 (d, J = 7.8 Hz, 1H), 7.71 (d, J = 7.6 Hz, 1H), 7.10-7.25 (m, 8H), 7.08 (br s, 1H), 6.96-7.02 (m, 2H), 6.66 (br s, 1H), 6.45 (d, J = 15.7 Hz, 1H), 6.16 (dt, J = 15.9, 5.8 Hz, 1H), 4.78 (ddd, J = 8.2, 8.2, 4.9 Hz, 1H), 4.31 (ddd, J = 11.3, 8.6, 2.9 Hz, 1H), 4.09 (ddd, J = 6.2, 6.2, 6.2 Hz, 1H), 3.88 (d, J = 4.9 Hz, 2H), 3.1-3.2 (m, 2H), 3.00 (dd, J = 13.8, 4.8 Hz, 1H), 2.84 (dd, J = 14.5, 2.6 Hz, 1H), 2.67-2.78 (m, 3H), 2.48-2.57 (m, 1H), 2.27-2.35 (m, 1H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 173.6, 172.1, 171.0, 170.2, 141.6, 138.0, 136.7, 130.1, 129.8, 128.7, 128.5, 128.4, 126.7, 126.2, 124.4, 62.3, 54.9, 54.4, 54.1, 37.5, 36.9, 35.8, 31.0. MS (ESI) Calculated for C₃₃H₃₇N₅O₅ [M+H]⁺: 584.3, found 584.3.

Cyclic-Ala-Phe-Ser-Val-Pro-Gly-Val-Trp-Ile-Ser-Tyr-Val (38):

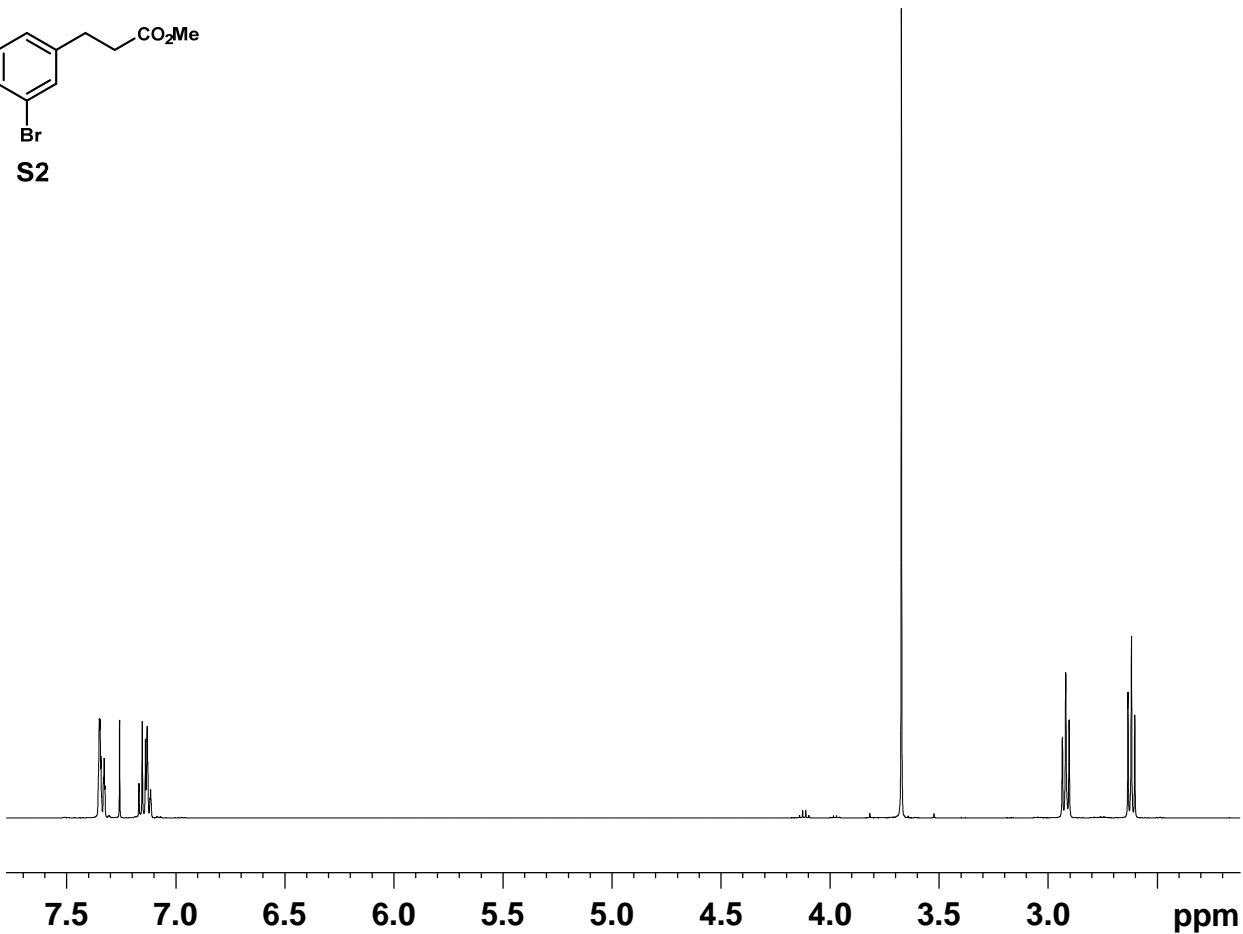
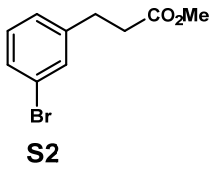
Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (10 mg, 0.007mmol, 66%). ¹H NMR (DMSO-d₆, 600 MHz): δ 10.67 (s, 1H), 8.24 (dd, J = 5.87 Hz, 1H), 8.09 (dd, J = 7.7 Hz, 1H), 8.02-8.08 (m, 3H), 8.01 (d, J = 7.9 Hz, 1H), 7.91 (d, J = 7.4 Hz, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.69-7.75 (m, 2H), 7.56-7.61 (m, 1H), 7.49-7.55 (m, 2H), 7.38 (d, J = 8.7 Hz, 1H), 7.31 (s, 1H), 7.23-7.28 (m, 3H), 7.13-7.22 (m, 5H), 7.10-7.13 (m, 3H), 7.05-7.09 (m, 3H), 6.99 (dd, J = 7.6, 7.6 Hz, 1H), 6.91 (dd, J = 7.5, 7.5 Hz, 1H), 6.78 (d, J = 8.3 Hz, 2H), 6.65 (d, J = 15.9 Hz, 1H), 6.42 (dt, J = 15.9, 5.8 Hz, 1H), 4.58 (d, J = 5.5 Hz, 2H), 4.53 (ddd, J = 8.5, 8.5, 5.4 Hz, 1H), 4.44-4.50 (m, 2H), 4.27-4.34 (m, 3H), 4.25

(dd, J = 7.6, 5.5 Hz, 1H), 4.14-4.20 (m, 2H), 4.05-4.13 (m, 3H), 3.75 (dd, J = 16.7, 6.1 Hz, 1H), 3.62-6.72 (m, 1H), 3.46-3.60 (m, 4H), 3.01-3.07 (m, 1H), 2.98 (dd, J = 13.7, 3.0 Hz, 1H), 2.87 (dd, J = 15.1, 9.6 Hz, 1H), 2.32-2.43 (m, 2H), 1.85-2.03 (m, 5H), 1.70-1.79 (m, 2H), 1.55-1.63 (m, 1H), 1.28-1.37 (m, 1H), 1.62 (d, J = 7 Hz, 3H), 0.94-1.0 (m, 1H), 0.85 (d, J = 6.6 Hz, 3H), 0.78-0.83 (m, 9H), 0.73 (d, J = 6.4 Hz, 3H), 0.63-0.72 (m, 6H), 0.67 (d, J = 6.8 Hz, 3H). ¹³C NMR (DMSO-d₆, 150 MHz, from HMBC/HSQC): δ 173.2, 172.45, 172.4, 172.3, 171.9, 171.4, 171.1, 171.07, 171.02, 170.5, 170, 169.9, 168.9, 157.1, 141.9, 137.9, 136.3, 133.2, 132.3, 131.6, 130.3, 129.1, 129, 127.9, 127.85, 127.8, 126.1, 126, 124.8, 124.1, 123.5, 120.7, 118.2, 118, 114.2, 111.1, 110.3, 67.9, 61.6, 61.5, 59.6, 57.9, 57.6, 56.8, 55.6, 54.9, 53.8, 53.6, 53.3, 48.7, 47, 42.3, 37.2, 37.1, 37, 36.4, 36.1, 30.6, 30.2, 29.3, 27.3, 24.5, 24.2, 22.1, 19.3, 19.1, 17.8, 17.5, 15.2, 11.1. MS (ESI) Calculated for C₇₈H₁₀₄N₁₄O₁₆[M+H]⁺: 1493.8, found 1493.7

Cyclic-Trp-Leu-Gln-Met-Thr-Gly-Phe-Tyr (39):

Following general procedure B, the corresponding compound was isolated by preparative HPLC (Waters Sunfire C18 30x150 mm) using a gradient of 35-100% CH₃CN/H₂O with 0.1% TFA. The fractions collected were combined and lyophilized (21 mg, 0.017mmol, 71%). ¹H NMR (DMSO-d₆, 500 MHz): δ 10.76 (d, J = 1.9 Hz, 1H), 8.11 (d, J = 7.8 Hz, 1H), 8.04-8.09 (m, 2H), 8.02 (d, J = 7.4 Hz, 1H), 7.96 (t, J = 5.4 Hz, 1H), 7.92 (d, J = 7.8 Hz, 1H), 7.81 (d, J = 7.9 Hz, 1H), 7.71 (d, J = 7.9 Hz, 1H), 7.55 (d, J = 7.8 Hz, 1H), 7.3 (d, J = 7.9 Hz, 1H), 7.23-7.27 (m, 3H), 7.17-7.23 (m, 6H), 7.12-7.17 (m, 3H), 7.06-7.10 (m, 2H), 7.01-7.05 (m, 2H), 6.95 (t, J = 7.5 Hz, 1H), 6.86 (d, J = 8.7 Hz, 2H), 6.72 (br. s, J = Hz, 1H), 6.66 (d, J = 15.9 Hz,

1H), 6.43 (dt, J = 15.9, 5.8 Hz, 1H), 4.61 (d, J = 5.4 Hz, 2H), 4.52 (ddd, J = 8.9, 8.9, 4.6 Hz, 1H), 4.45 (ddd, J = 8.4, 8.4, 5.0 Hz, 1H), 4.4 (ddd, J = 8.1, 8.1, 5.0 Hz, 1H), 4.35 (ddd, J = 8.9, 8.9, 4.0 Hz, 1H), 4.13-4.25 (m, 3H), 3.93-3.99 (m, 1H), 3.69 (dd, J = 17.1, 5.7 Hz, 1H), 3.56 (dd, J = 16.8, 5.2 Hz, 1H), 3.1 (dd, J = 14.9, 4.8 Hz, 1H), 2.99 (dd, J = 13.8, 4.2 Hz, 1H), 2.87-2.96 (m, 2H), 2.64-2.78 (m, 4H), 2.31-2.45 (m, 4H), 1.85-1.98 (m, 5H), 1.69-1.83 (m, 2H), 1.00 (d, J = 6.4 Hz, 3H), 0.75-0.86 (m, 6H). ¹³C NMR (DMSO-d₆, 125 MHz): δ 174.2, 173.4, 172.3, 172.3, 172.1, 171.53, 171.51, 171.3, 170.7, 168.8, 157.3, 142.1, 138.2, 136.6, 136.5, 132.7, 130.7, 130.4, 129.7, 129.1, 128.5, 128.2, 127.8, 126.8, 126.7, 125.4, 124.6, 123.9, 121.3, 118.8, 118.7, 114.7, 111.8, 110.6, 68.4, 67.1, 58.8, 54.6, 54.5, 54.2, 52.9, 52.4, 51.6, 42.3, 41.0, 38.0, 37.2, 37.1, 32.2, 31.9, 31.3, 29.9, 29.2, 27.6, 24.5, 23.6, 22.0, 20.0, 15.0. MS (ESI) Calculated for C₆₃H₇₉N₁₁O₁₂S [M+H]⁺: 1214.6, found 1214.2.



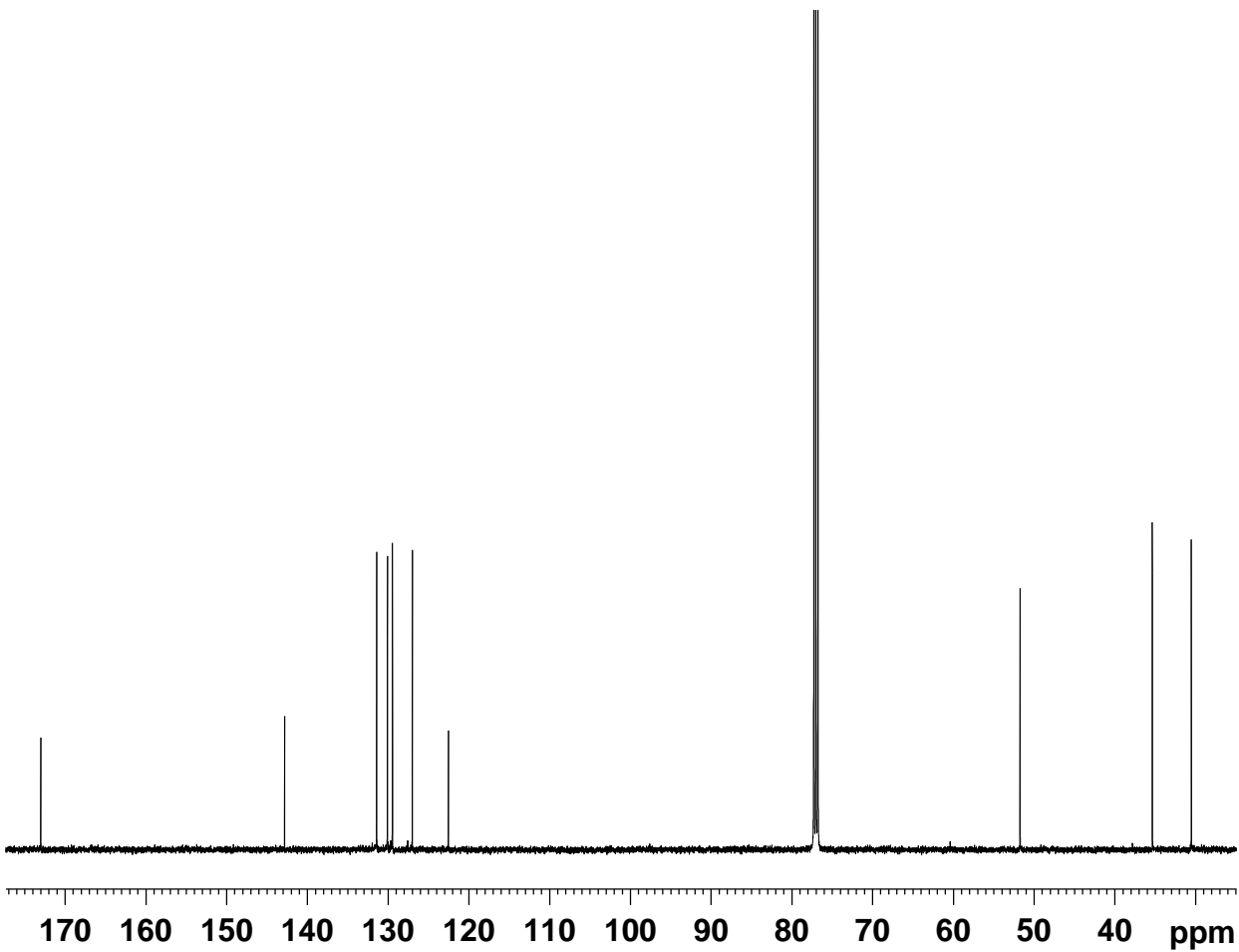
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Current Data Parameters
NAME          KL-5-56
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20130112
Time          15.42
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            17.27
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          500.1330008 MHz
NUC1          1H
P1            10.00 usec
PLW1          13.5000000 W

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

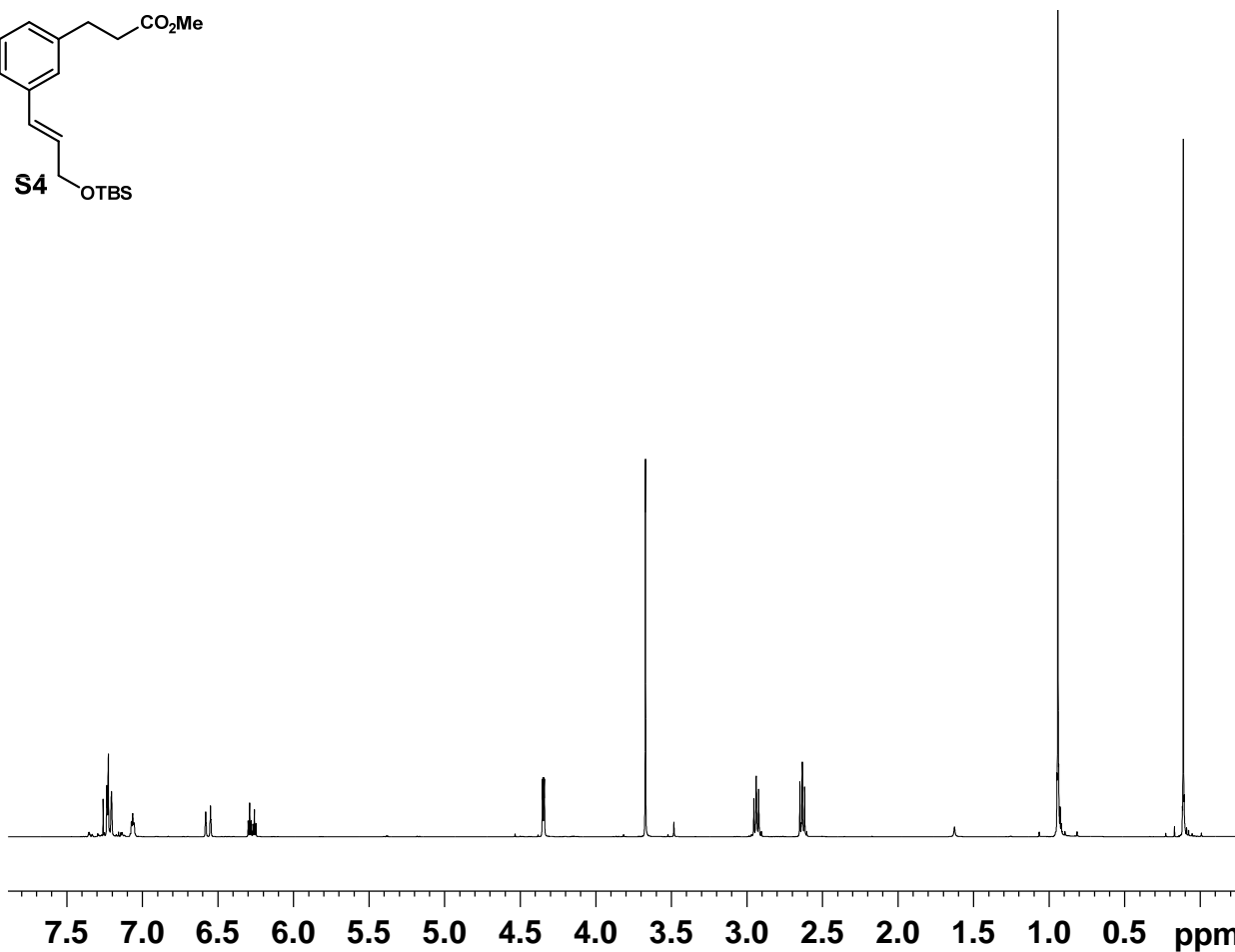
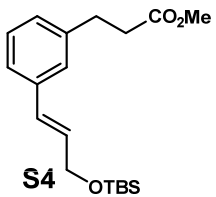
Current Data Parameters
NAME          KL-5-56
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20130112
Time          15.44
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            22
DS            2
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG            202.91
DW            16.000 usec
DE            18.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          125.7722511 MHz
NUC1          13C
P1            9.63 usec
PLW1          23.0000000 W

===== CHANNEL f2 =====
SFO2          500.1330008 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          13.5000000 W
PLW12         0.21094000 W
PLW13         0.13500001 W

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

```

Current Data Parameters
NAME      KL-4-117
EXPNO    1
PROCNO   1

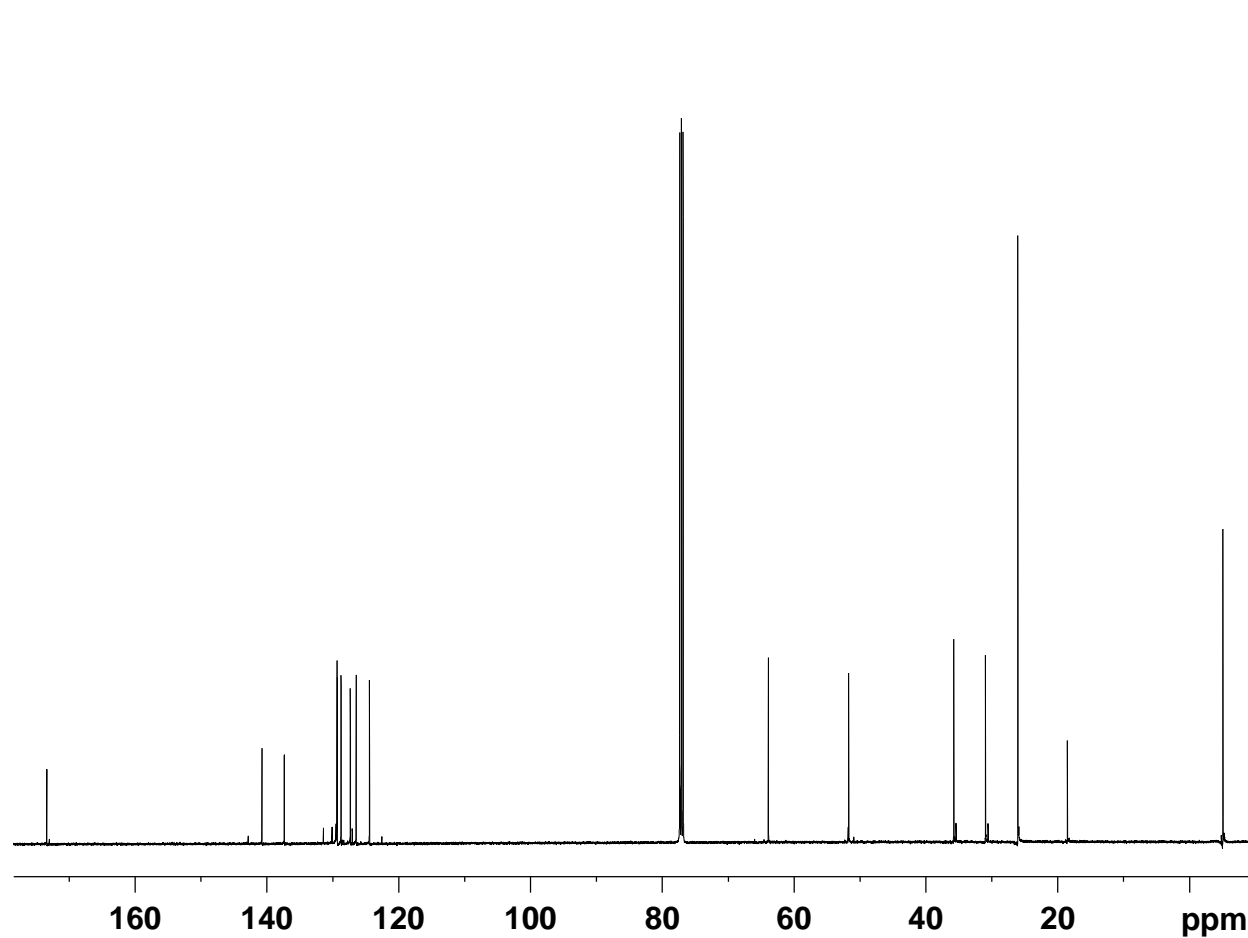
F2 - Acquisition Parameters
Date_    20120219
Time     13.45
INSTRUM  av500
PROBHD   5 mm DCH 13C-1
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       11
DW       50.000 usec
DE       10.00 usec
TE       296.0 K
D1       2.0000000 sec
TD0      1
  
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       10.00 usec
PLW1     13.5000000 W
SFO1     500.1330008 MHz
  
```

```

F2 - Processing parameters
SI       65536
SF       500.1300146 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

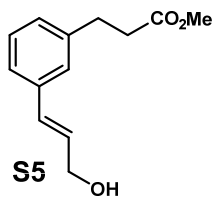


```

Current Data Parameters
NAME      KL-4-117
EXPNO    2
PROCNO   1
  
```

```

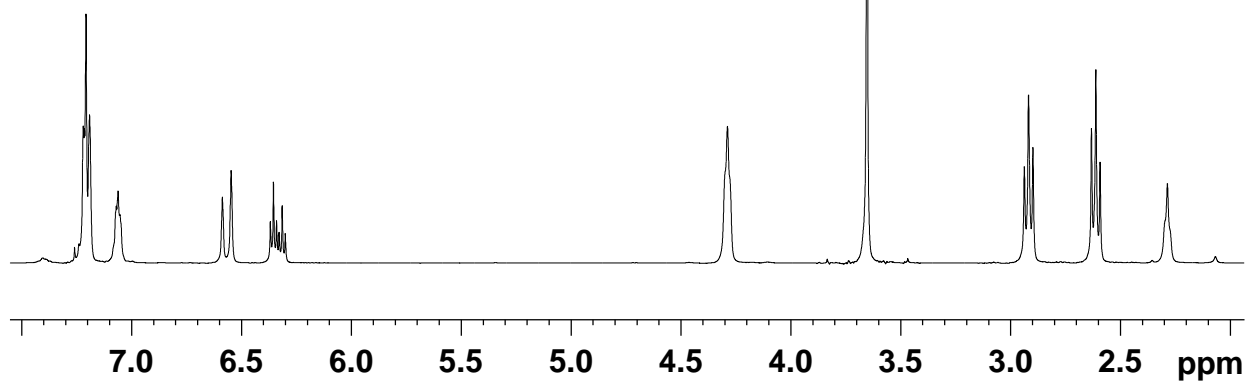
F2 - Processing parameters
SI       131072
SF       125.7577892 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```



Current Data Parameters
 NAME KL-4-122_aftcol
 EXPNO 374
 PROCNO 1

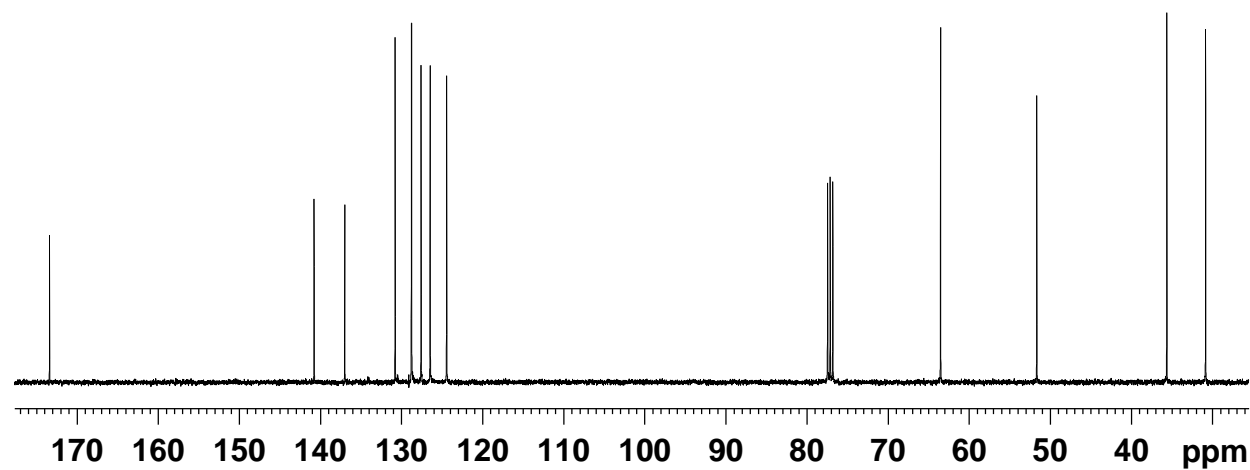
F2 - Acquisition Parameters
 Date_ 20120213
 Time 19.53
 INSTRUM arx400
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8064.516 Hz
 FIDRES 0.123055 Hz
 AQ 4.0632820 sec
 RG 180
 DW 62.000 usec
 DE 88.57 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 9.00 usec
 SF01 400.1324008 MHz
 NUCLEUS 1H

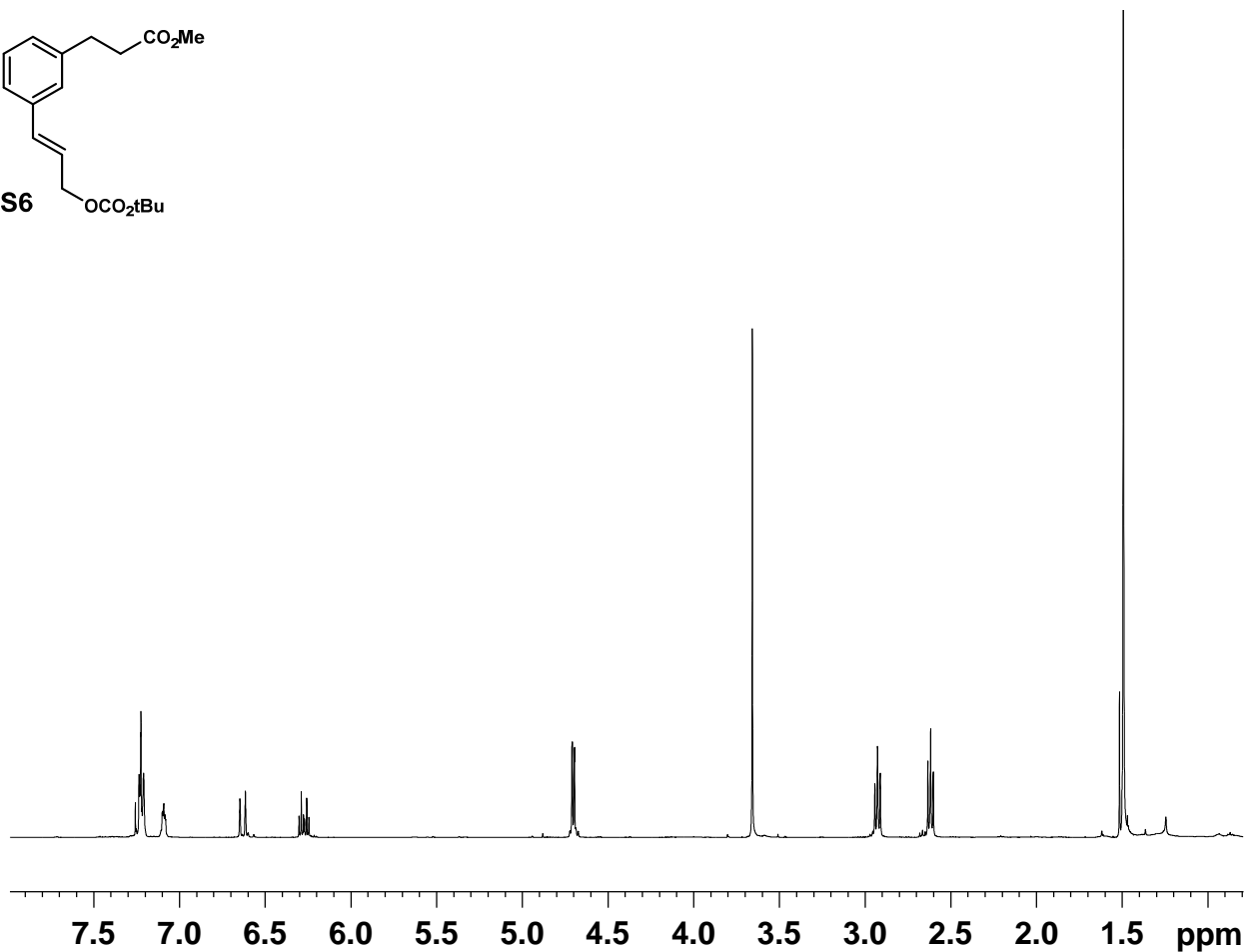
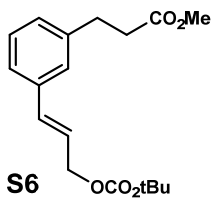
F2 - Processing parameters
 SI 65536
 SF 400.1300173 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-4-122_aftcol
 EXPNO 375
 PROCNO 1

F2 - Processing parameters
 SI 65536
 SF 100.6127710 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





```

Current Data Parameters
NAME          KL-4-125
EXPNO         1
PROCNO        1

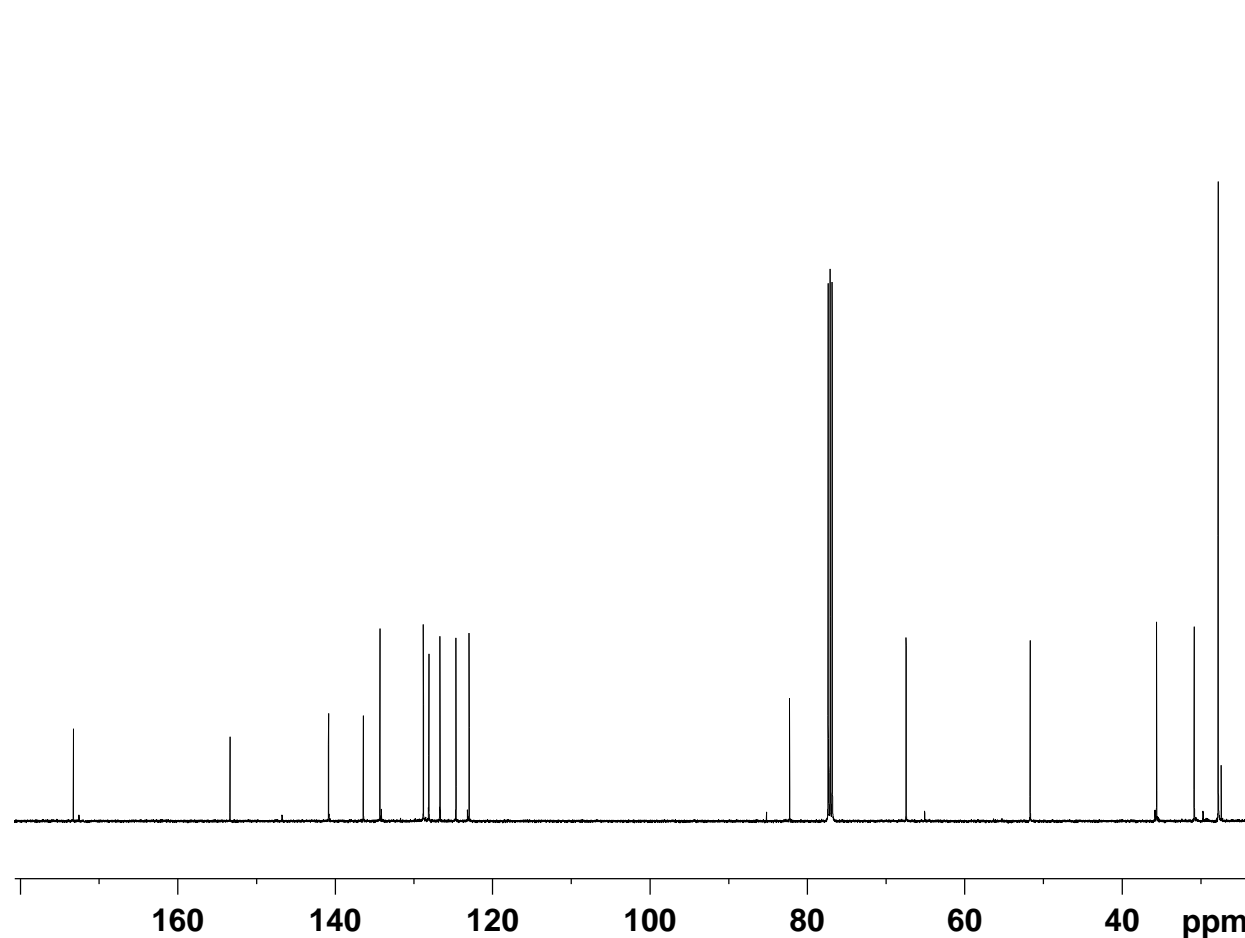
F2 - Acquisition Parameters
Date_         20120227
Time          19.53
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            29.99
DW            50.000 usec
DE            10.00 usec
TE            296.0 K
D1            2.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            10.00 usec
PLW1          13.5000000 W
SF01          500.1330008 MHz
  
```

```

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

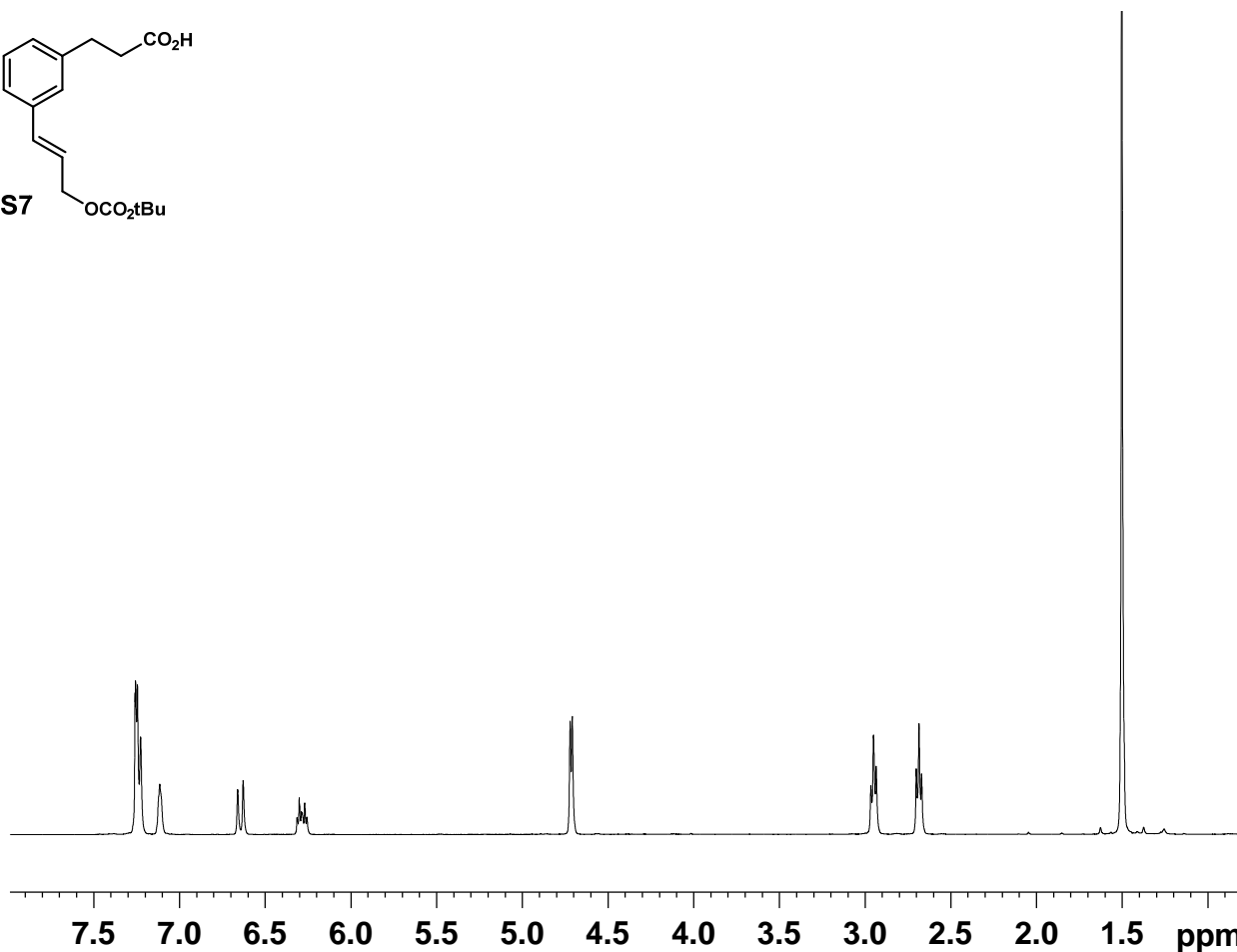
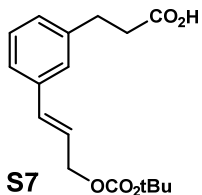


```

Current Data Parameters
NAME          KL-4-125
EXPNO         2
PROCNO        1
  
```

```

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



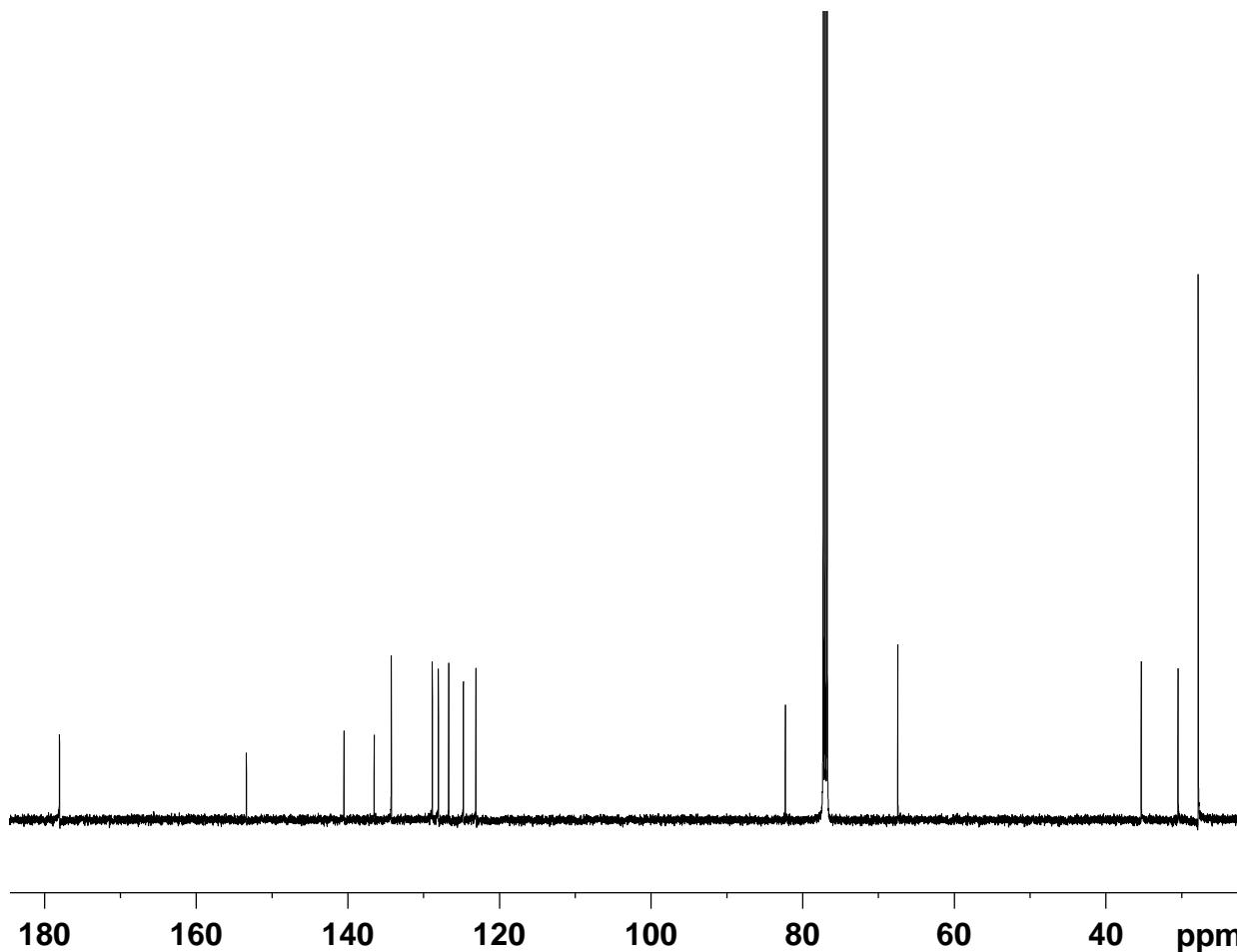
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Current Data Parameters
NAME          KL-5-60
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20130124
Time          11.25
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            11
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          500.1330008 MHz
NUC1          1H
P1            10.00 usec
PLW1          13.5000000 W

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

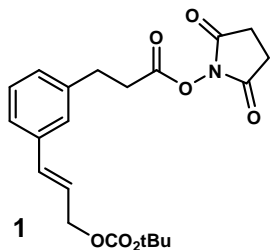
Current Data Parameters
NAME          KL-5-60
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20130124
Time          11.29
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            32
DS            2
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG            202.91
DW            16.000 usec
DE            18.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          125.7722511 MHz
NUC1          13C
P1            9.63 usec
PLW1          23.0000000 W

===== CHANNEL f2 =====
SFO2          500.1330008 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          13.5000000 W
PLW12         0.21094000 W
PLW13         0.13500001 W

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

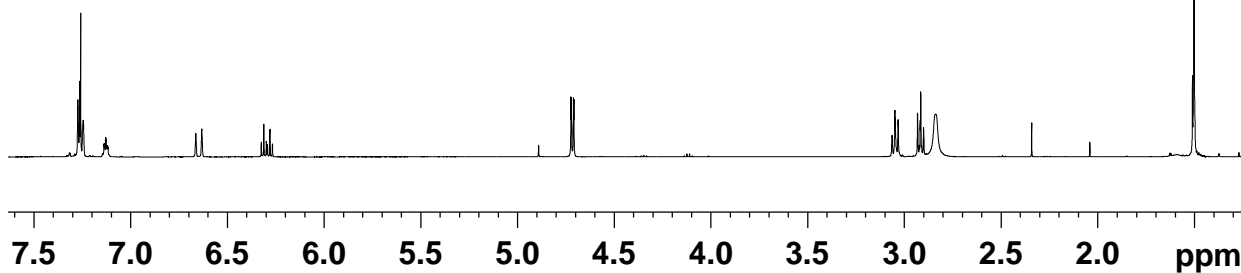


Current Data Parameters
 NAME KL-5-55
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130124
 Time 15.36
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 11
 DW 50.000 usec
 DE 10.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 13.5000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



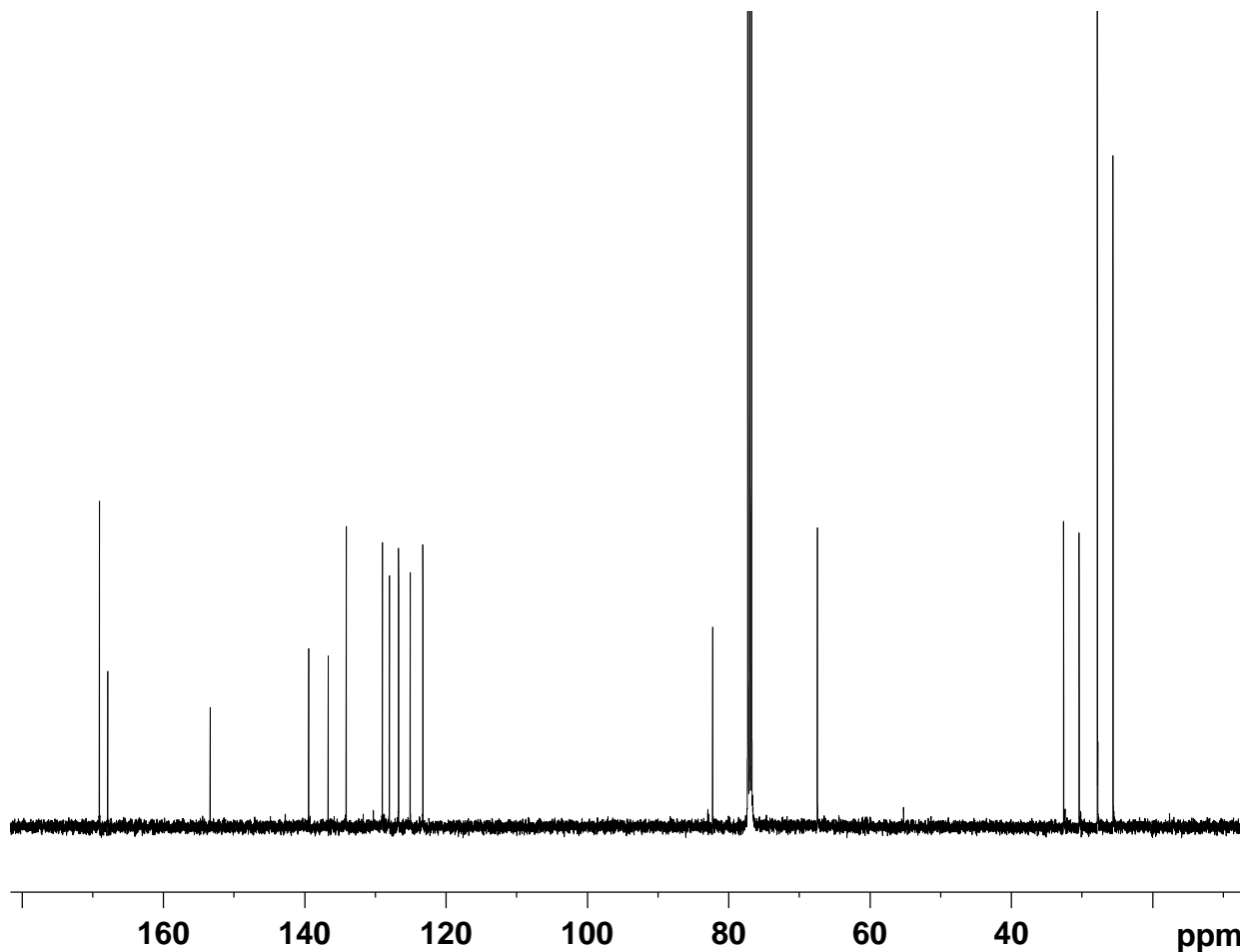
Current Data Parameters
 NAME KL-5-55
 EXPNO 2
 PROCNO 1

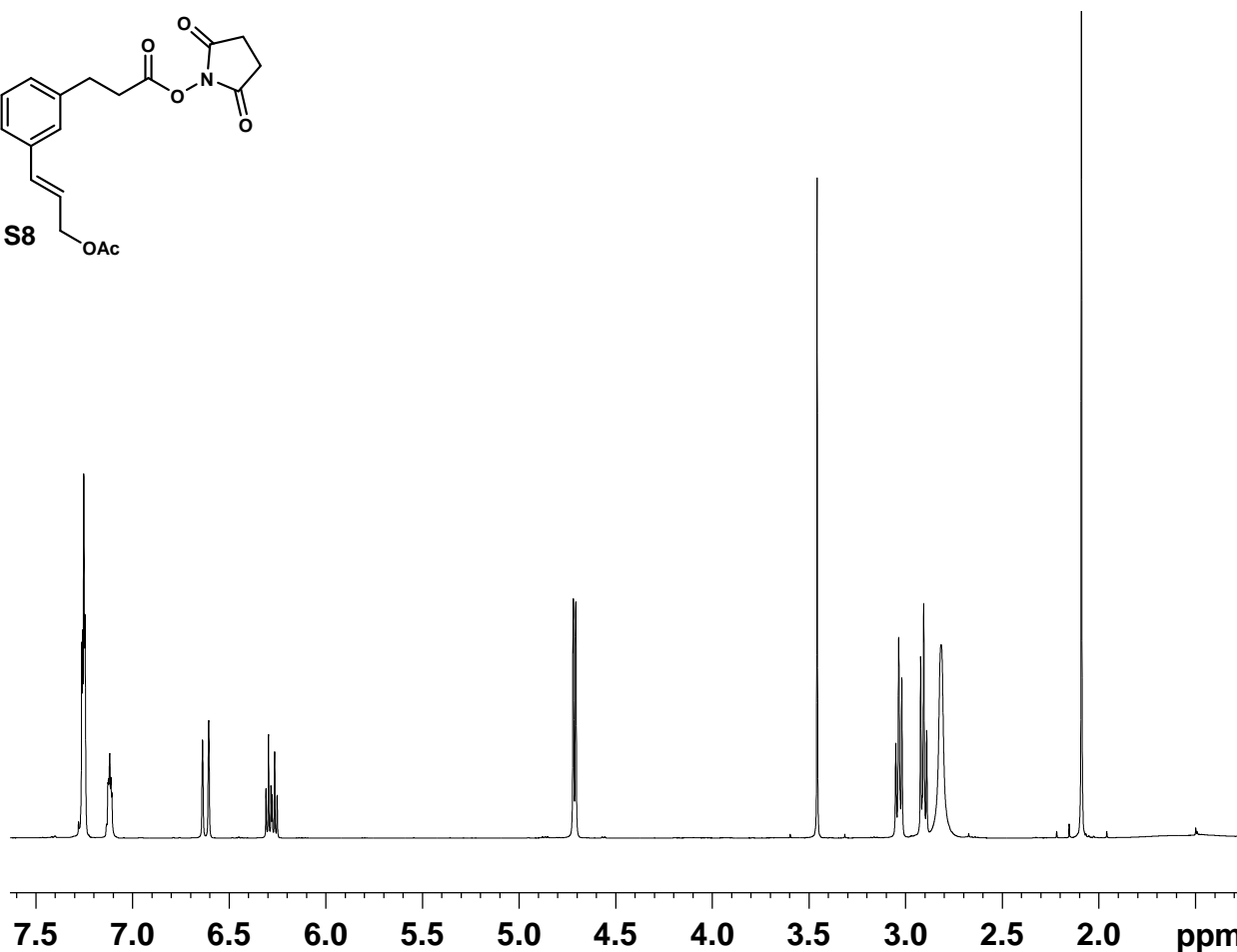
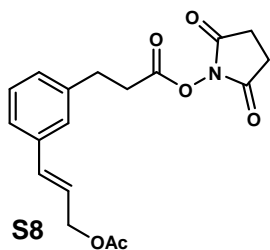
F2 - Acquisition Parameters
 Date_ 20130124
 Time 15.37
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 31
 DS 2
 SWH 31250.000 Hz
 FIDRES 0.476837 Hz
 AQ 1.0485760 sec
 RG 202.91
 DW 16.000 usec
 DE 18.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7722511 MHz
 NUC1 13C
 P1 9.63 usec
 PLW1 23.0000000 W

==== CHANNEL f2 =====
 SFO2 500.1330008 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.5000000 W
 PLW12 0.21094000 W
 PLW13 0.13500001 W

F2 - Processing parameters
 SI 131072
 SF 125.7577892 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





```

Current Data Parameters
NAME          HI_OAc
EXPNO         1
PROCNO        1

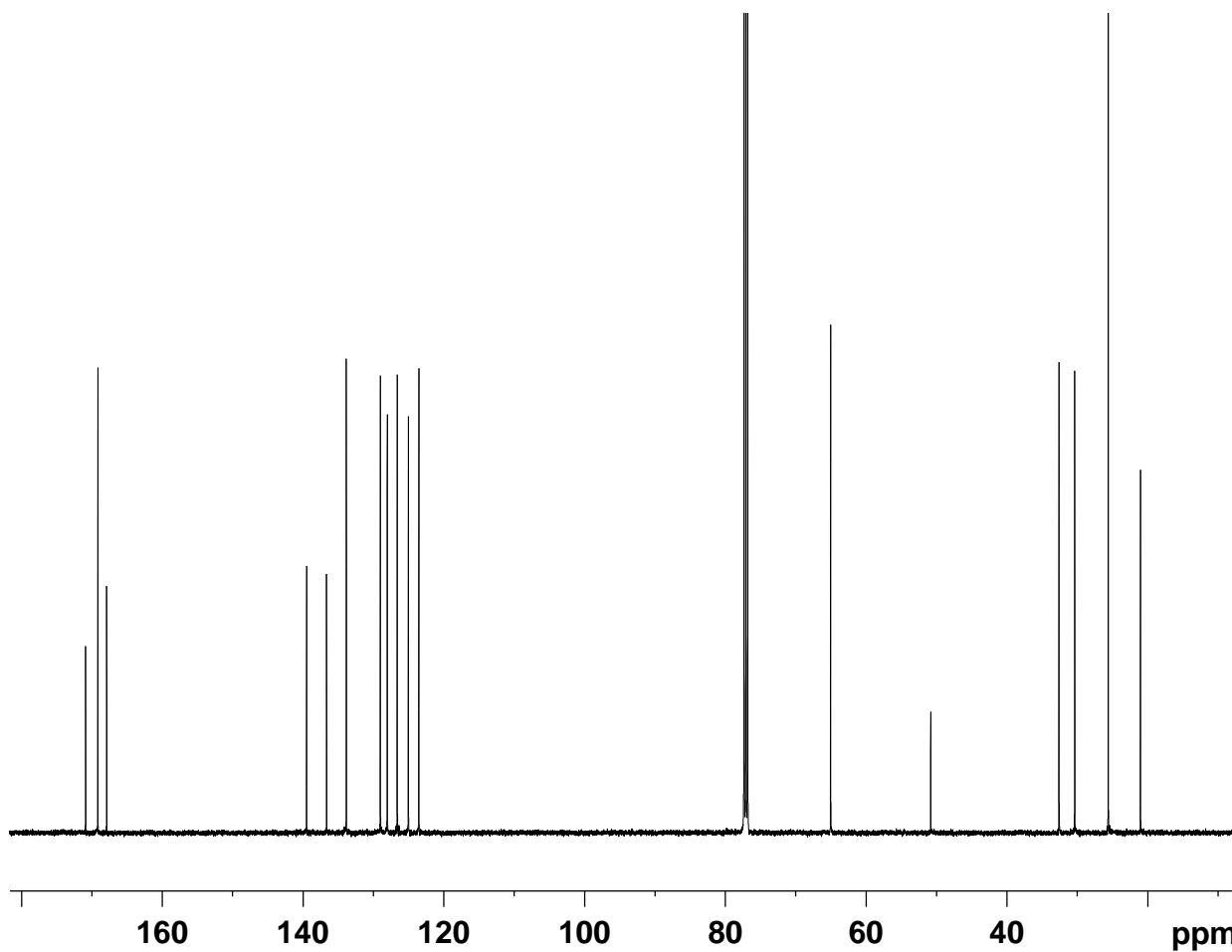
F2 - Acquisition Parameters
Date_         20130424
Time          12.07
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            11
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
SFO1          500.1330008 MHz
NUC1          1H
P1            10.00 usec
PLW1          13.5000000 W
  
```

```

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

Current Data Parameters
NAME          HI_OAc
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20130424
Time          12.09
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            31
DS            2
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG            202.91
DW            16.000 usec
DE            18.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
SFO1          125.7722511 MHz
NUC1          13C
P1            9.63 usec
PLW1          23.0000000 W
  
```

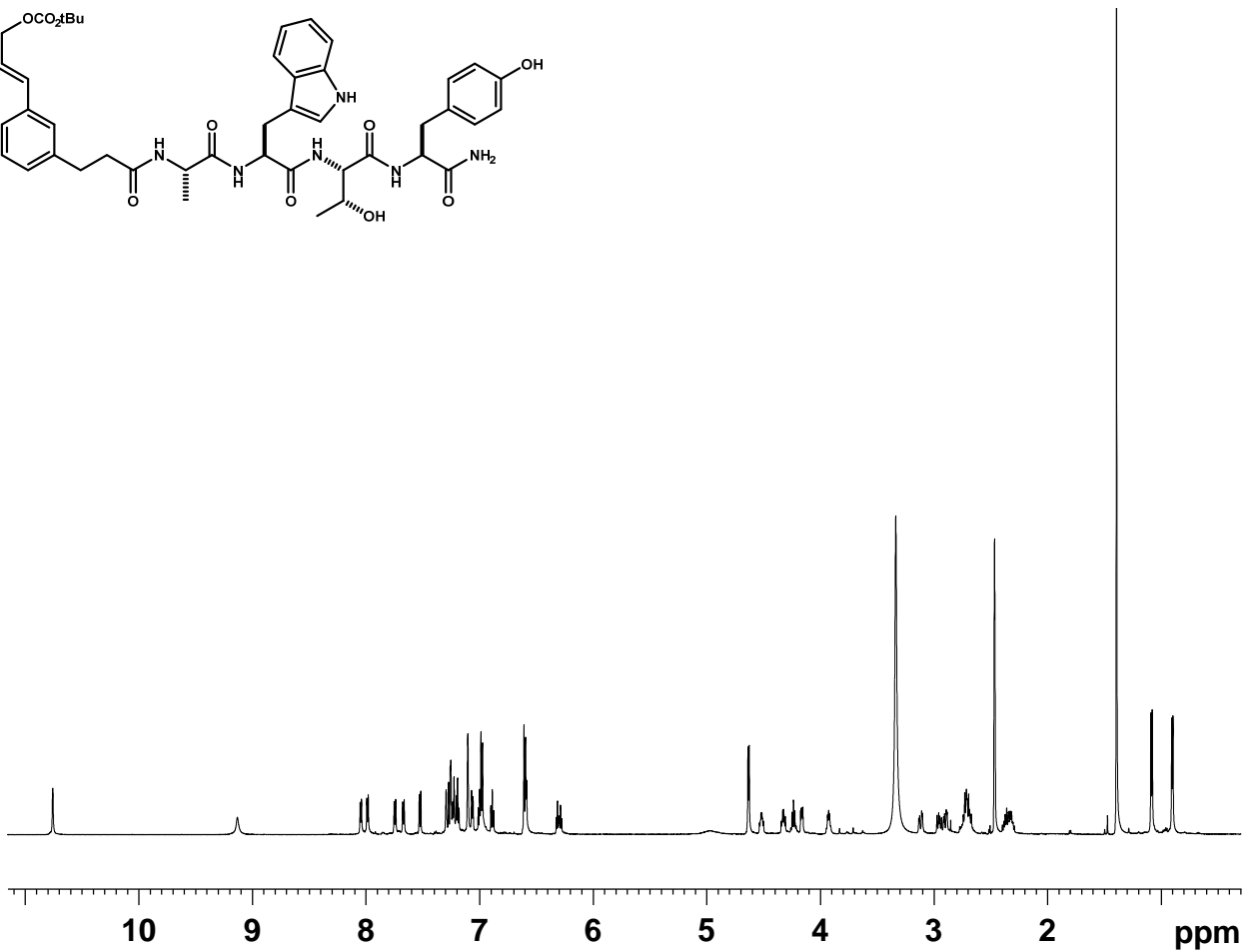
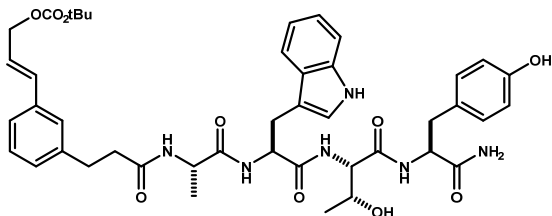
```

===== CHANNEL f2 =====
SFO2          500.1330008 MHz
NUC2          1H
CPDPRG[2]    waltz16
PCPD2         80.00 usec
PLW2          13.5000000 W
PLW12         0.21094000 W
PLW13         0.13500001 W
  
```

```

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00
  
```

Acyclic-Ala-Trp-Thr-Tyr (2):



```

Current Data Parameters
NAME          KL-4-38
EXPNO         1
PROCNO        1

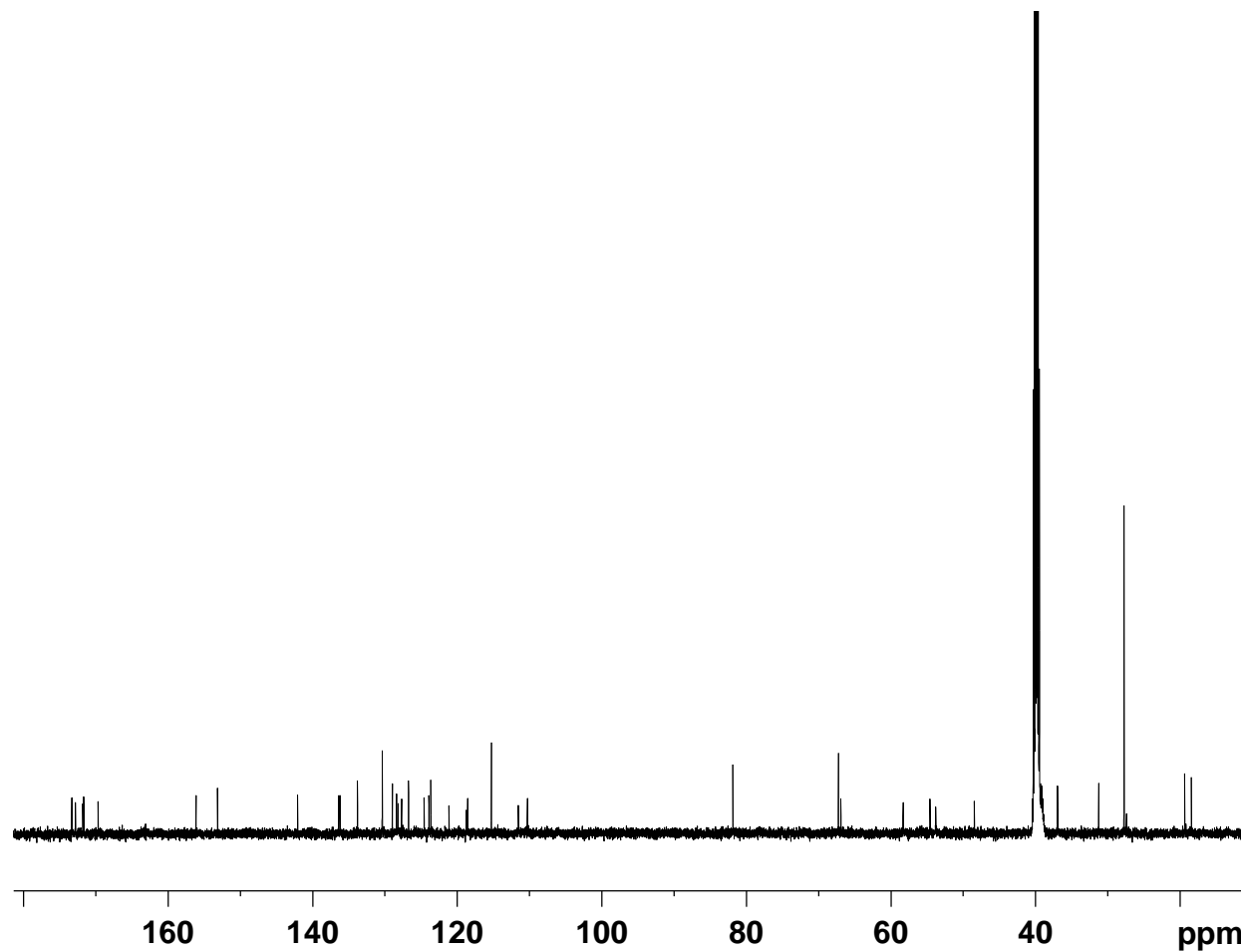
F2 - Acquisition Parameters
Date_         20111012
Time          18.07
INSTRUM       av600
PROBHD        5 mm BB5
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           12376.237 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            181
DW            40.400 usec
DE            6.50 usec
TE            295.2 K
D1            2.0000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.00 usec
PL1           -1.00 dB
PL1W          31.62277603 W
SFO1          600.1336008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            600.1300273 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



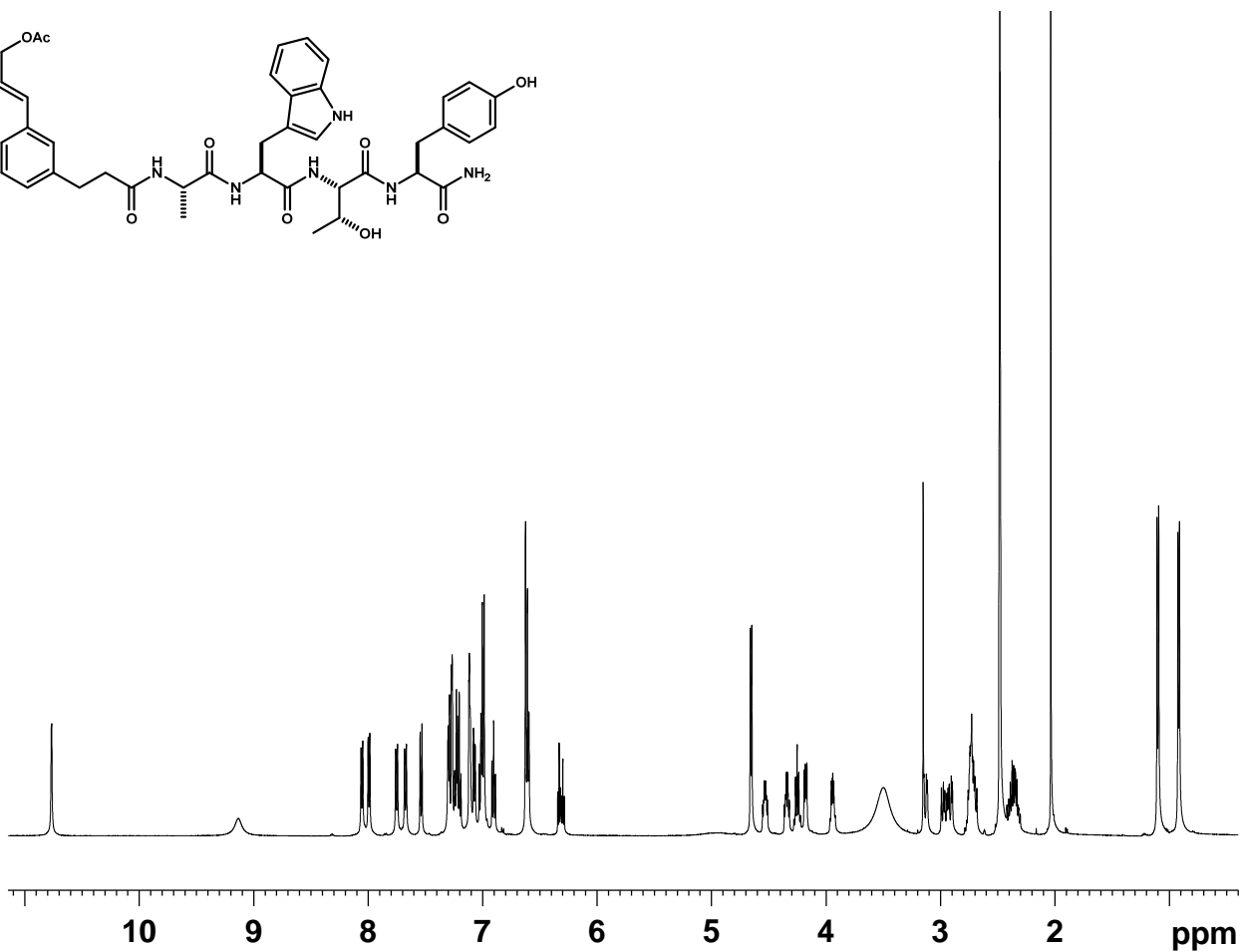
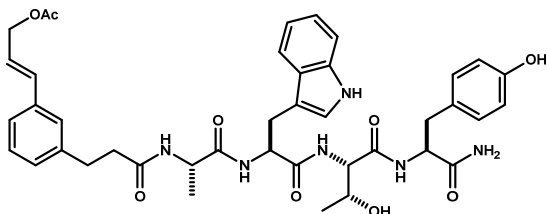
```

Current Data Parameters
NAME          KL-4-38
EXPNO         2
PROCNO        1
    
```

```

F2 - Processing parameters
SI            65536
SF            150.9028319 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

Acyclic-Ala-Trp-Thr-Tyr (3):



```

Current Data Parameters
NAME          KL-5-144b
EXPNO         1
PROCNO        1

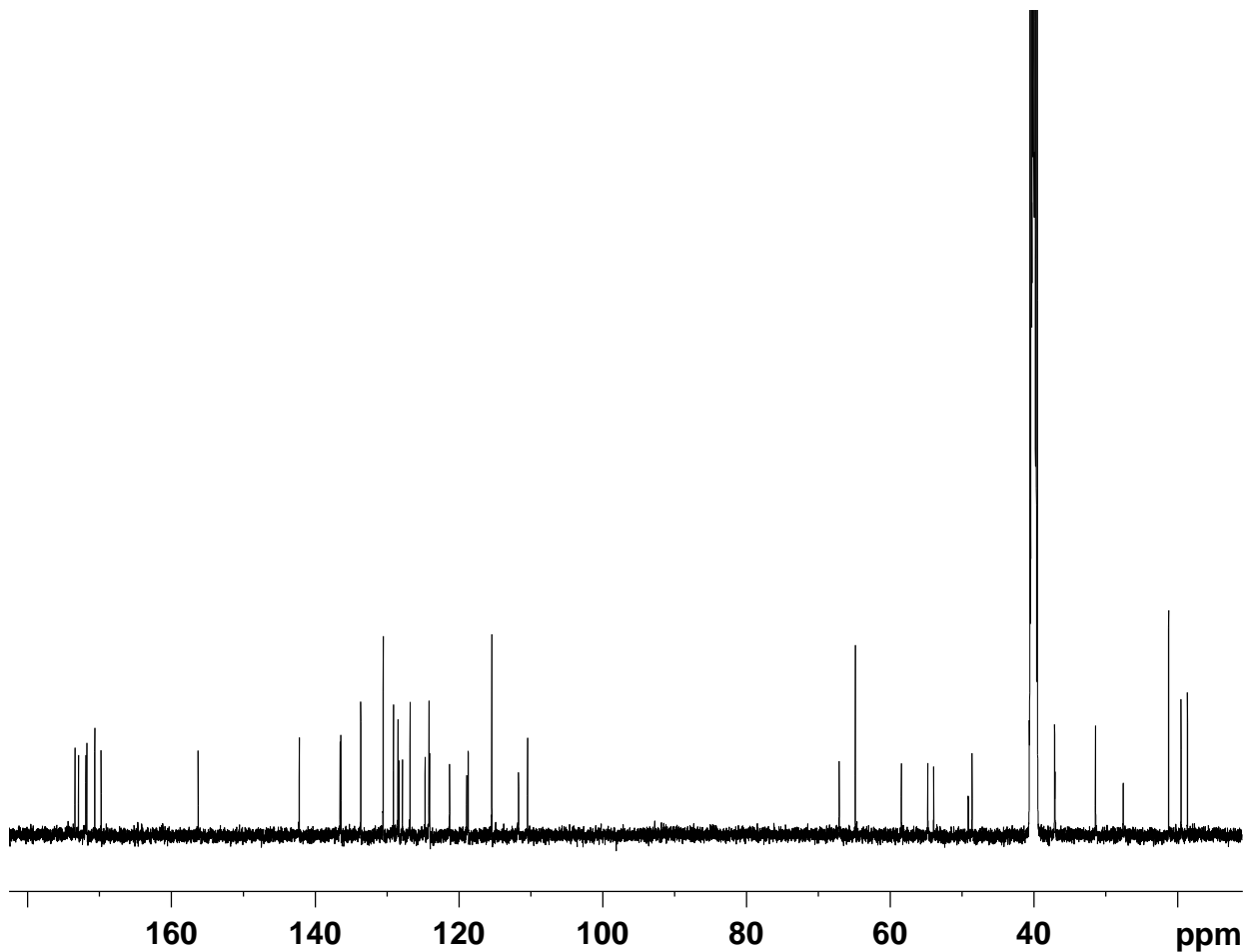
F2 - Acquisition Parameters
Date_         20130321
Time          18.13
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            11
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
SFO1          500.1330008 MHz
NUC1          1H
P1            10.00 usec
PLW1          13.5000000 W
    
```

```

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



```

Current Data Parameters
NAME          KL-5-144b
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20130321
Time          18.16
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            92
DS            2
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG            202.91
DW            16.000 usec
DE            18.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
SFO1          125.7722511 MHz
NUC1          13C
P1            9.63 usec
PLW1          23.0000000 W
    
```

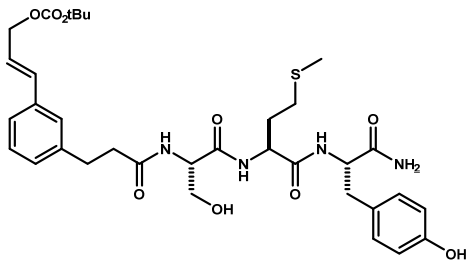
```

===== CHANNEL f2 =====
SFO2          500.1330008 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          13.5000000 W
PLW12         0.2109400 W
PLW13         0.13500001 W
    
```

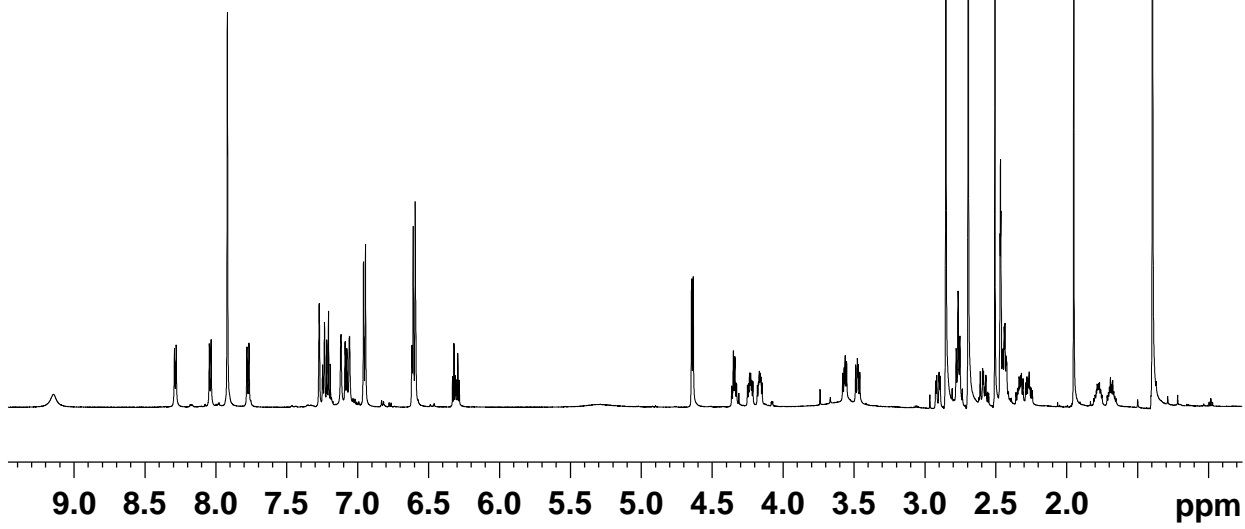
```

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

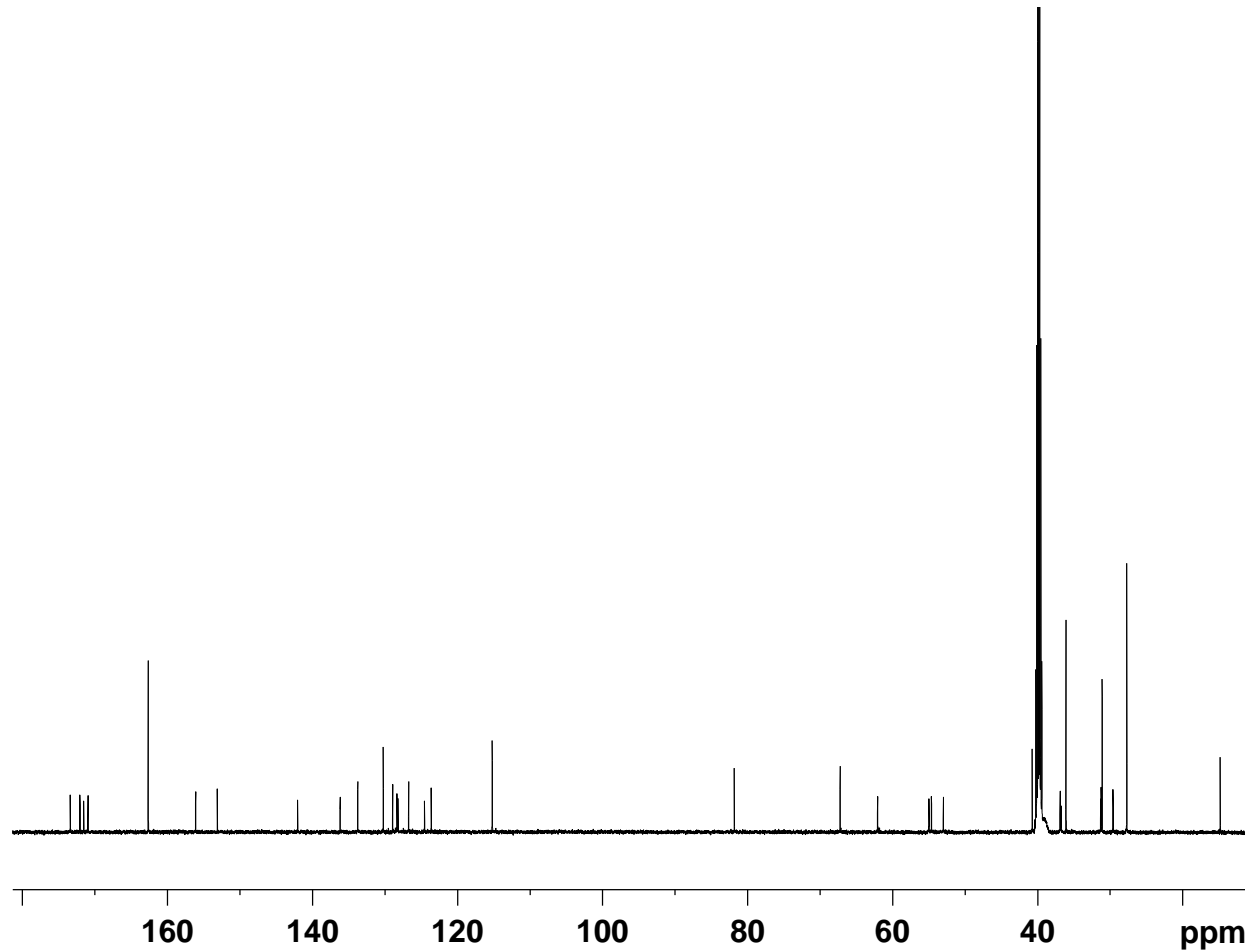

Acyclic-Ser-Met-Tyr (S9):



Current Data Parameters
 NAME KL-III-288
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110831
 Time 15.21
 INSTRUM av600
 PROBHD 5 mm BB5
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 12376.237 Hz
 FIDRES 0.188846 Hz
 AQ 2.6476543 sec
 RG 114
 DW 40.400 usec
 DE 6.50 usec
 TE 294.6 K
 D1 2.0000000 sec
 TD0 1

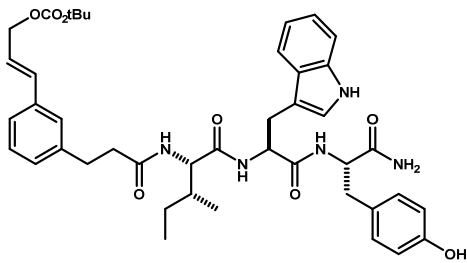


==== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -1.00 dB
 PL1W 31.62277603 W
 SFO1 600.1336008 MHz
 F2 - Processing parameters
 SI 65536
 SF 600.1300273 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



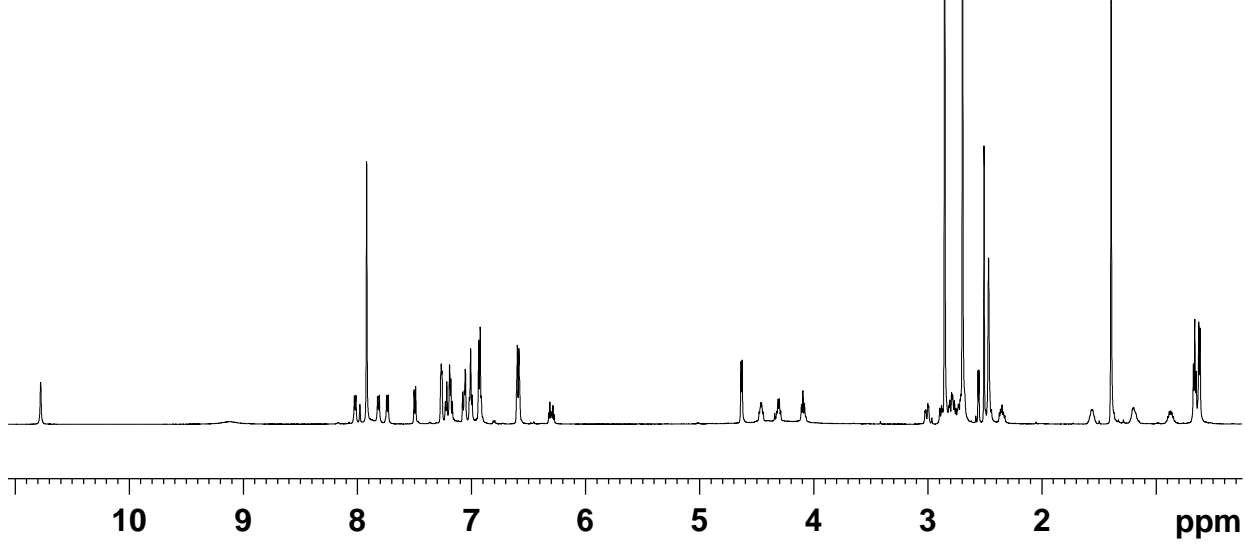
Current Data Parameters
 NAME KL-III-288
 EXPNO 2
 PROCNO 1
 F2 - Processing parameters
 SI 65536
 SF 150.9028319 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Acyclic-Ile-Trp-Tyr (S10):



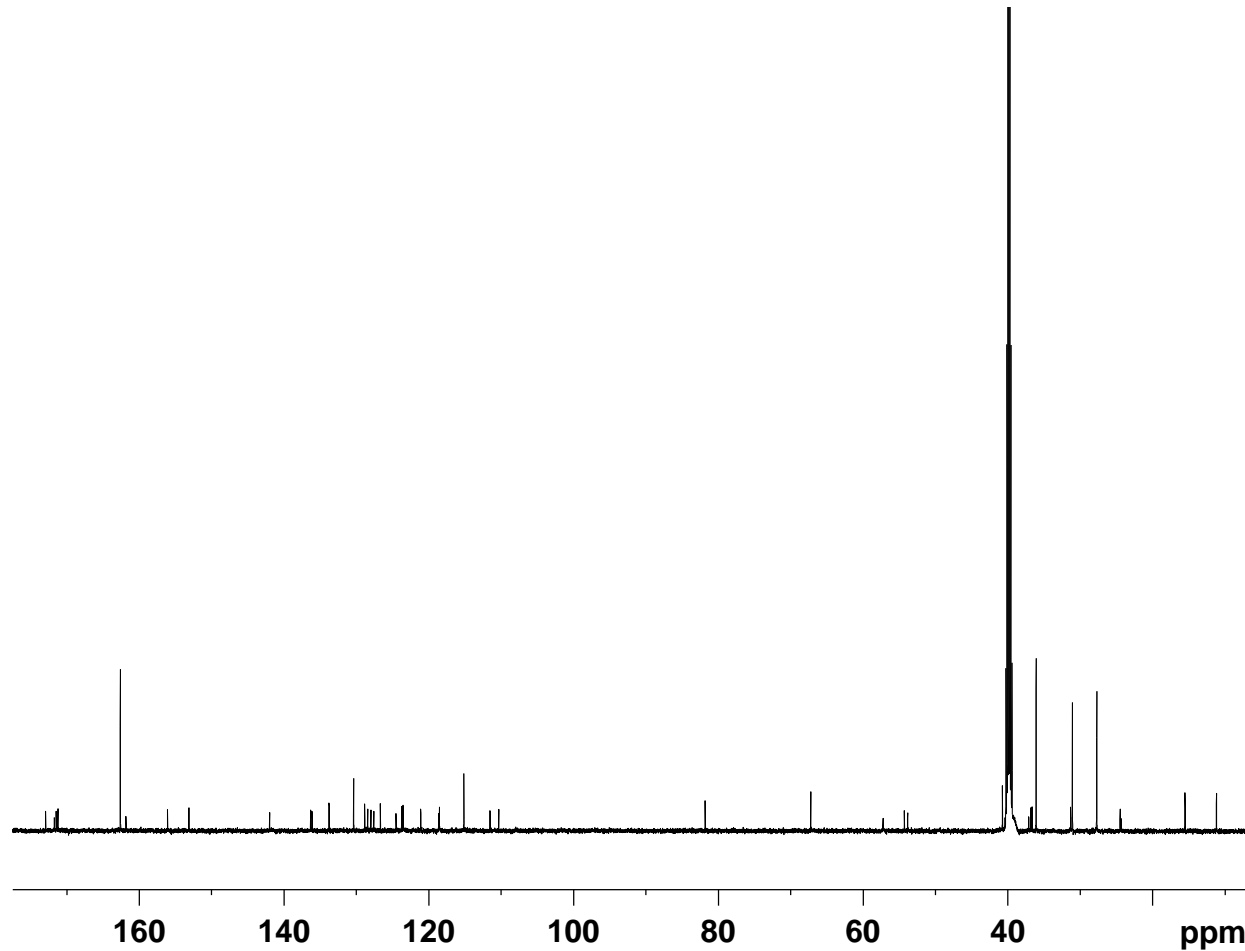
Current Data Parameters
 NAME KL-III-287
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110828
 Time 18.29
 INSTRUM av600
 PROBHD 5 mm BB5
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 12376.237 Hz
 FIDRES 0.188846 Hz
 AQ 2.6476543 sec
 RG 90.5
 DW 40.400 usec
 DE 6.50 usec
 TE 294.1 K
 D1 2.0000000 sec
 TD0 1



==== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -1.00 dB
 PL1W 31.62277603 W
 SFO1 600.1336008 MHz

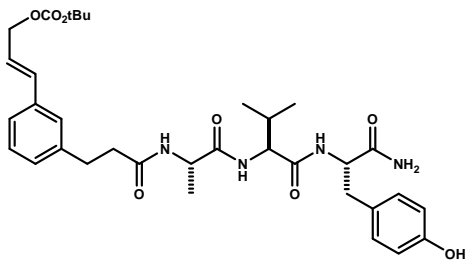
F2 - Processing parameters
 SI 65536
 SF 600.1300273 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-III-287
 EXPNO 2
 PROCNO 1

F2 - Processing parameters
 SI 65536
 SF 150.9028319 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

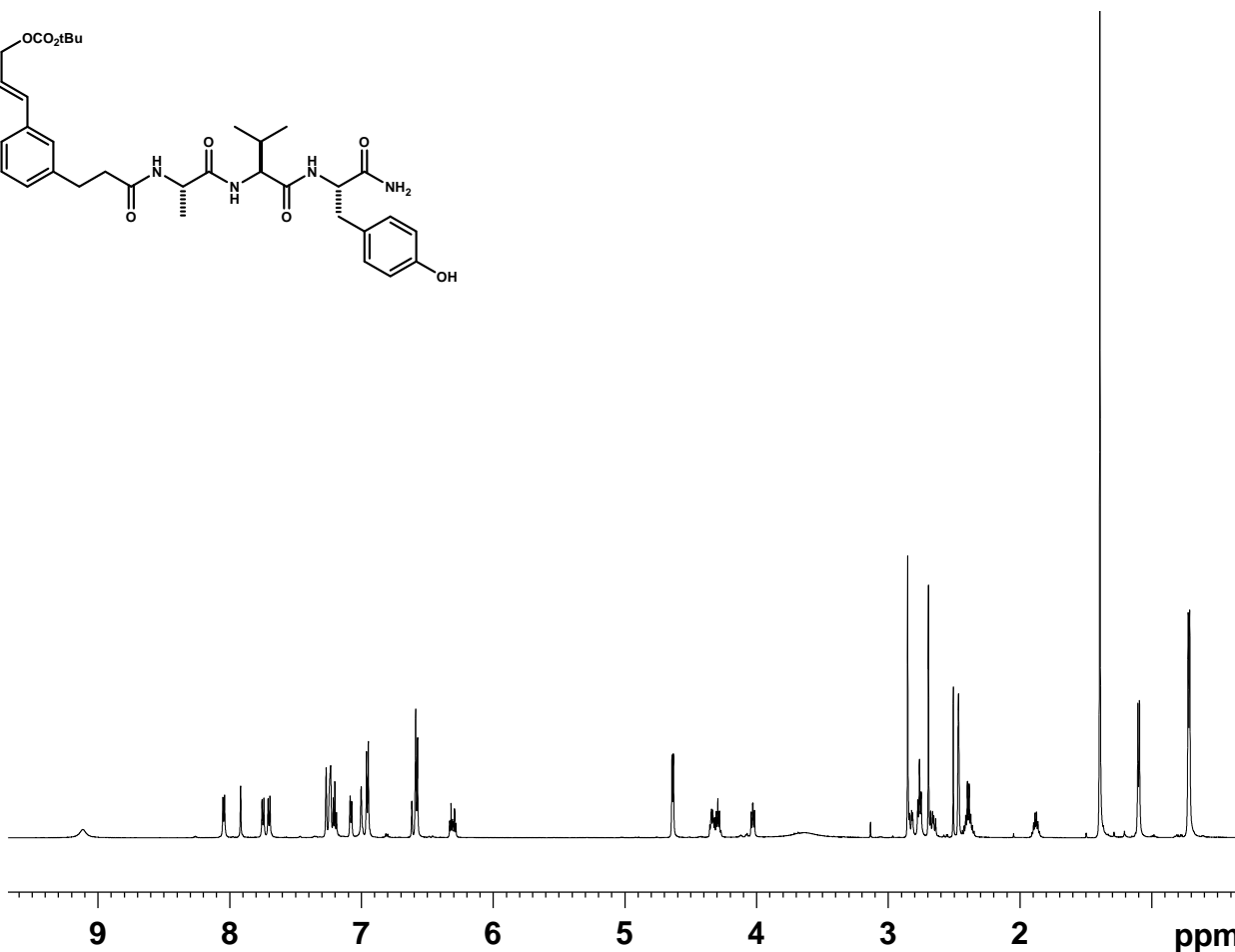
Acyclic-Ala-Val-Tyr (S11):



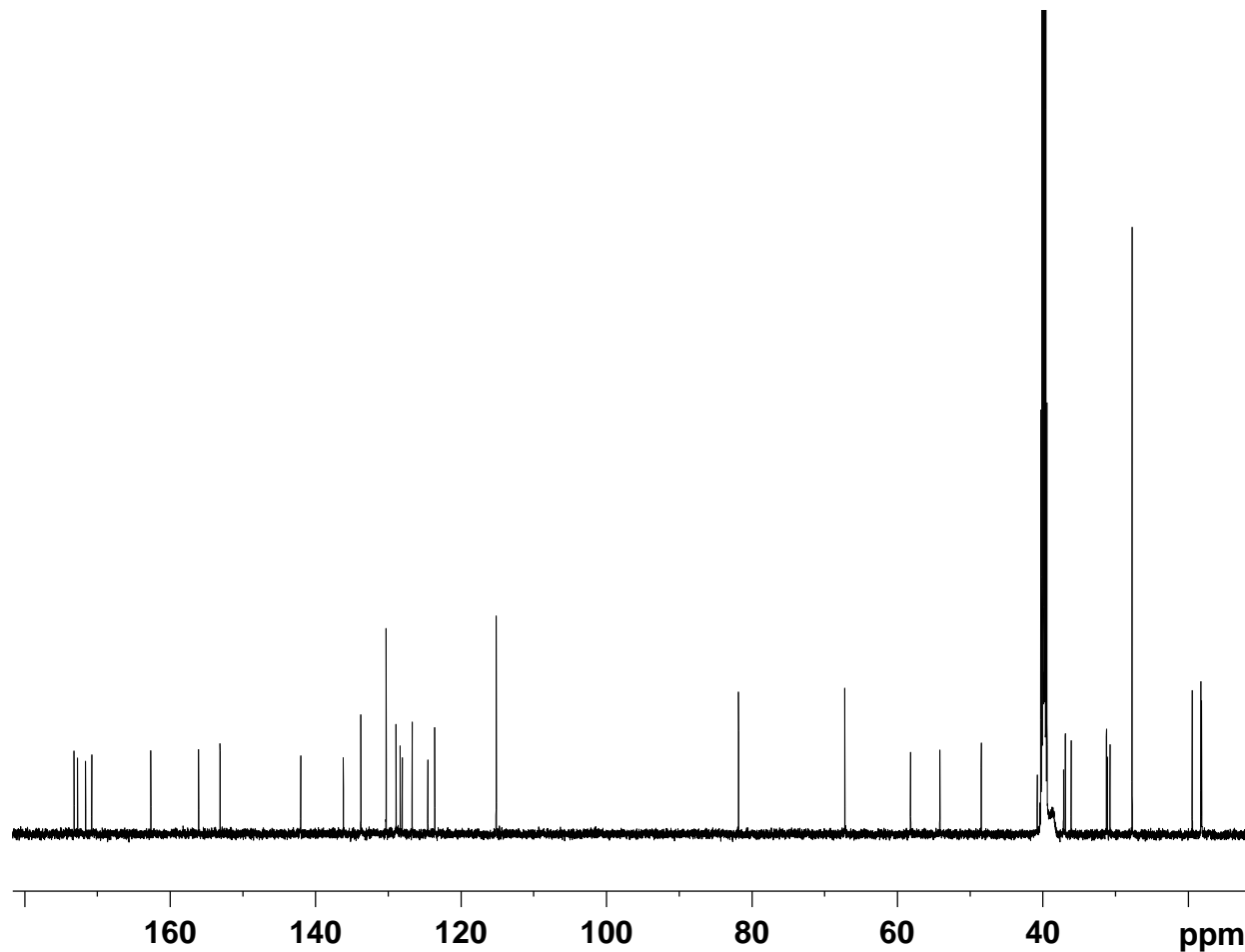
Current Data Parameters
 NAME KL-III-286
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110829
 Time 13.37
 INSTRUM av600
 PROBHD 5 mm BB5
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 12376.237 Hz
 FIDRES 0.188846 Hz
 AQ 2.6476543 sec
 RG 114
 DW 40.400 usec
 DE 6.50 usec
 TE 294.3 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -1.00 dB
 PL1W 31.62277603 W
 SFO1 600.1336008 MHz

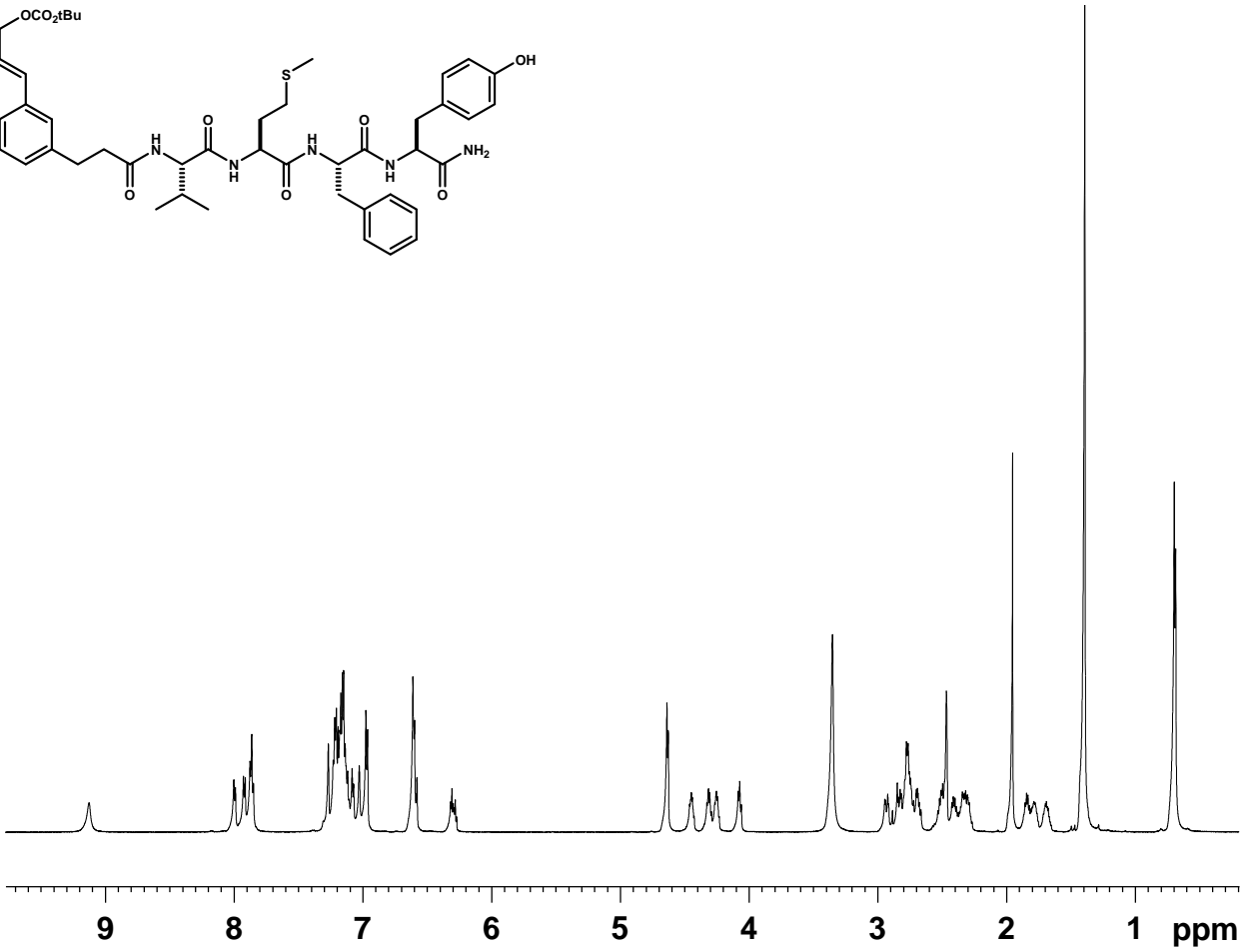
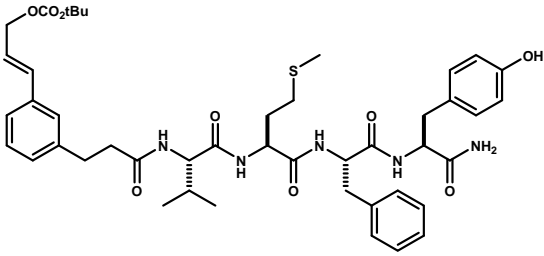
F2 - Processing parameters
 SI 65536
 SF 600.1300273 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-III-286
 EXPNO 2
 PROCNO 1
 F2 - Processing parameters
 SI 65536
 SF 150.9028319 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Acyclic-Val-Met-Phe-Tyr (S12):



```

Current Data Parameters
NAME          KL-4-39
EXPNO         2
PROCNO        1

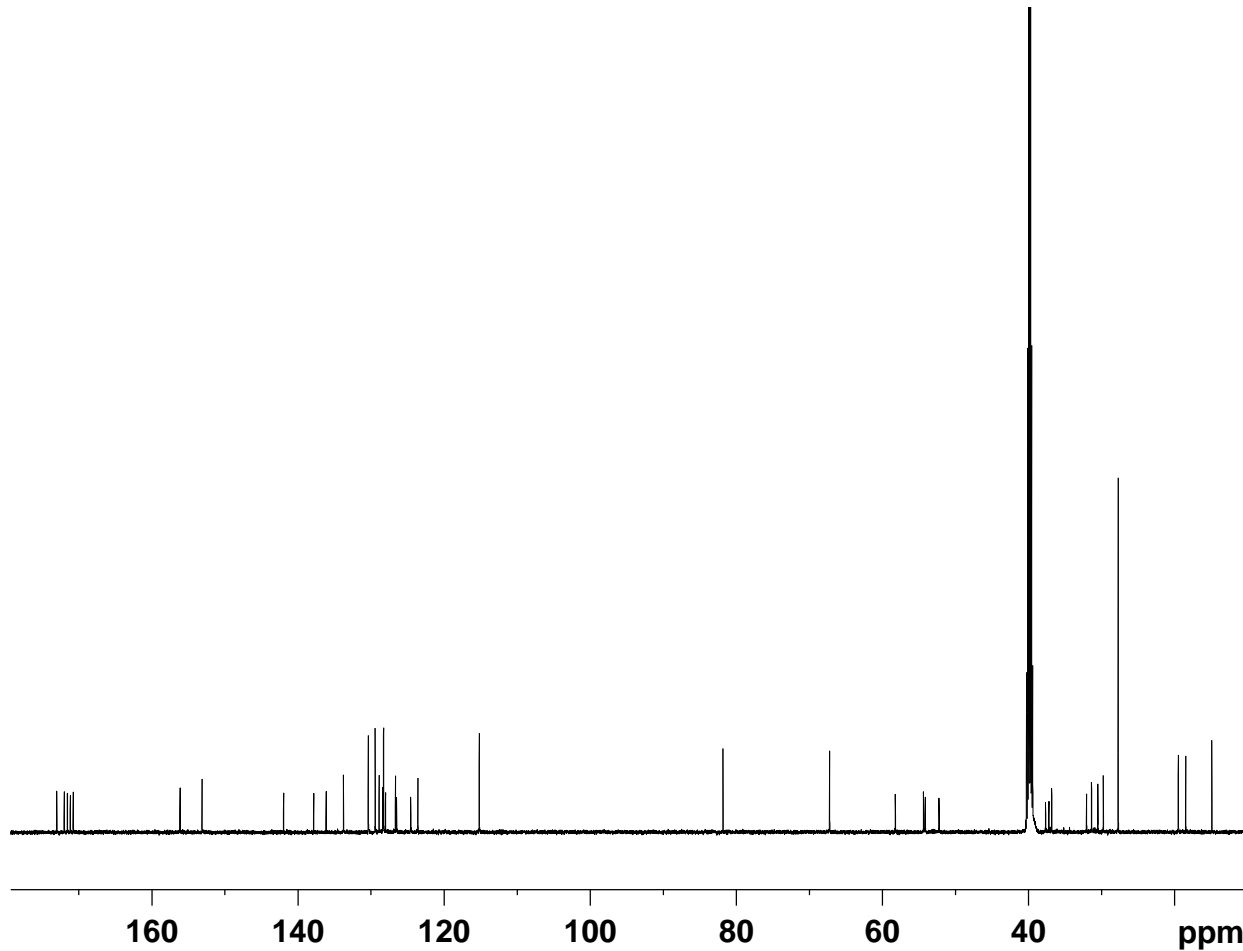
F2 - Acquisition Parameters
Date_         20111010
Time          19.06
INSTRUM       av600
PROBHD        5 mm BB5
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            2
DS            0
SWH           12376.237 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            90.5
DW            40.400 usec
DE            6.50 usec
TE            294.7 K
D1            2.0000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.00 usec
PL1           -1.00 dB
PL1W          31.62277603 W
SFO1          600.1336008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            600.1300273 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



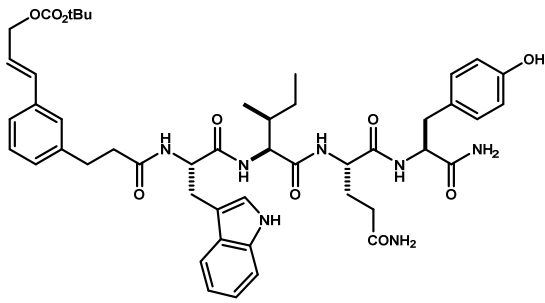
```

Current Data Parameters
NAME          KL-4-39
EXPNO         3
PROCNO        1
    
```

```

F2 - Processing parameters
SI            65536
SF            150.9028319 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

Acyclic-Trp-Ile-Gln-Tyr (S13):



```

Current Data Parameters
NAME          KL-III-294
EXPNO         1
PROCNO        1

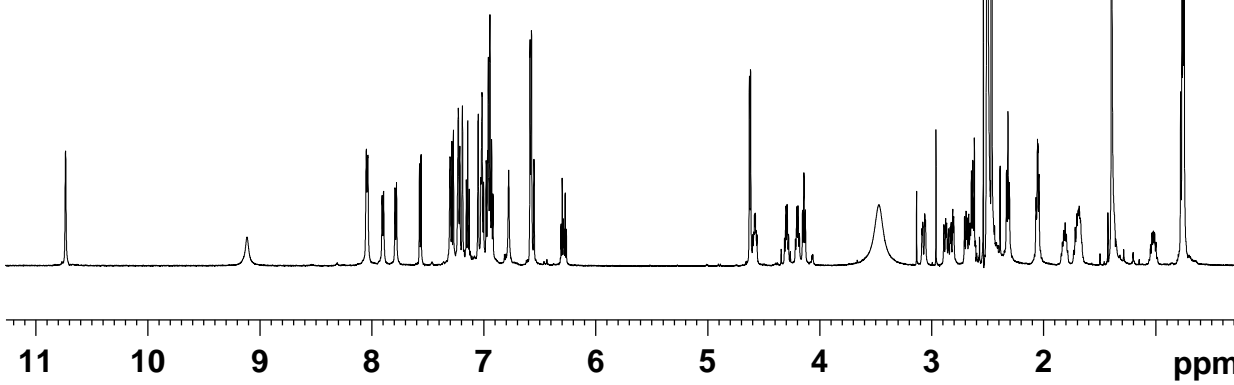
F2 - Acquisition Parameters
Date_         20110831
Time          14.13
INSTRUM       av600
PROBHD        5 mm BB5
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           12376.237 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            114
DW            40.400 usec
DE            6.50 usec
TE            294.0 K
D1            2.0000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.00 usec
PL1           -1.00 dB
PL1W          31.62277603 W
SF01          600.1336008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            600.1300273 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

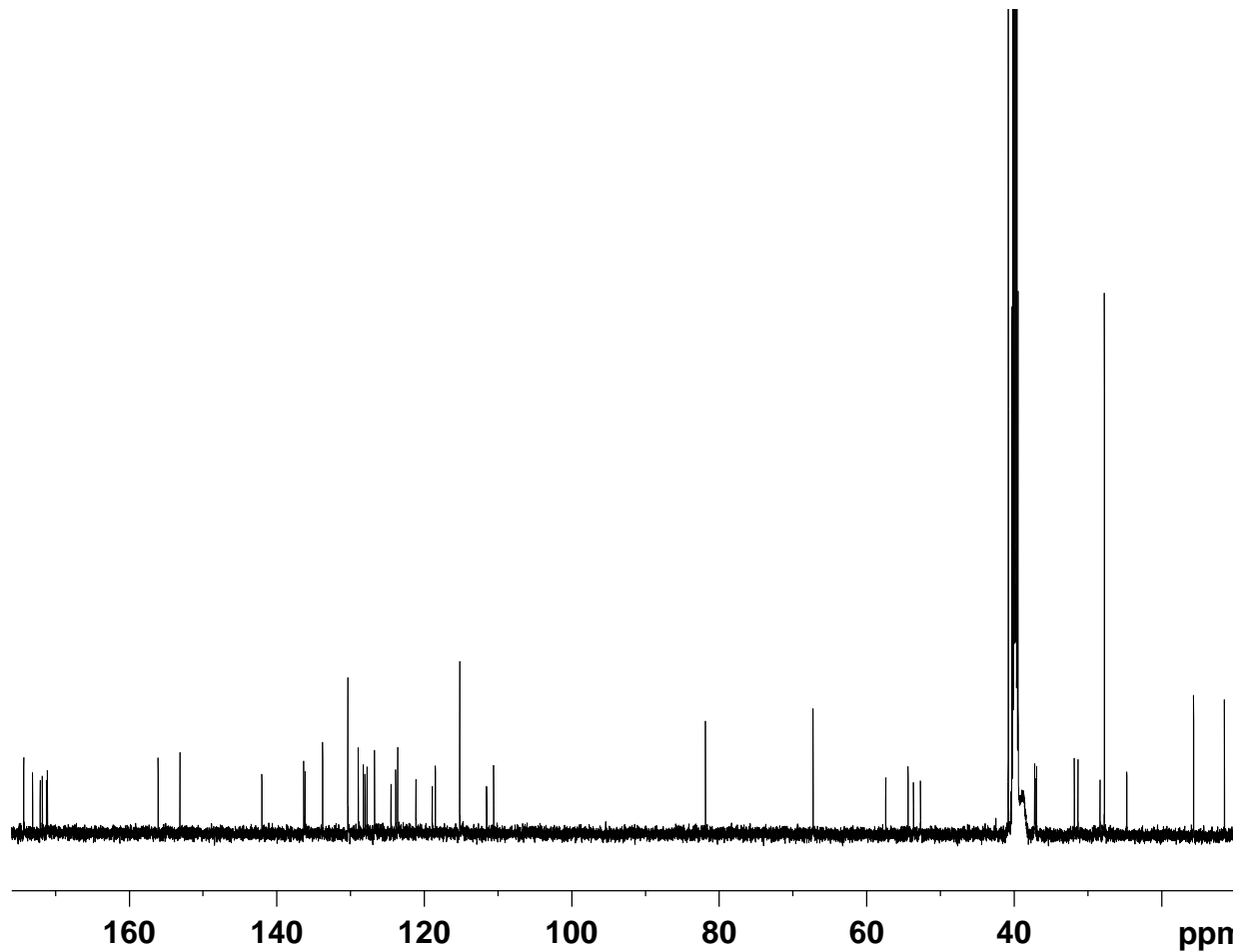


```

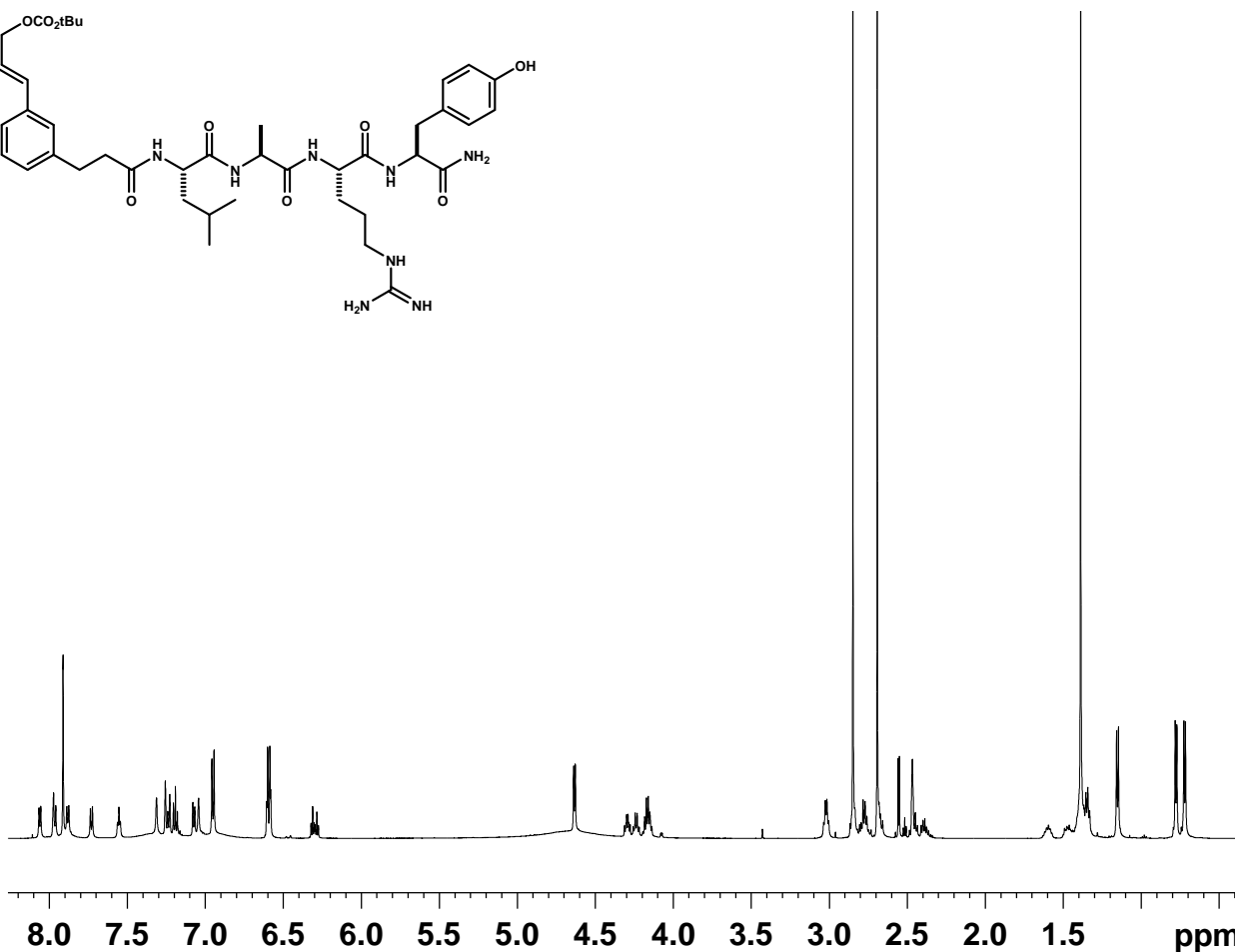
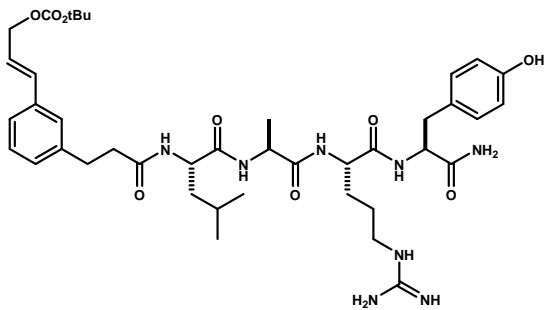
Current Data Parameters
NAME          KL-III-294
EXPNO         2
PROCNO        1
    
```

```

F2 - Processing parameters
SI            65536
SF            150.9028319 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```



Acyclic-Leu-Ala-Arg-Tyr (S14):



```

Current Data Parameters
NAME          KL-4-8
EXPNO         1
PROCNO        1

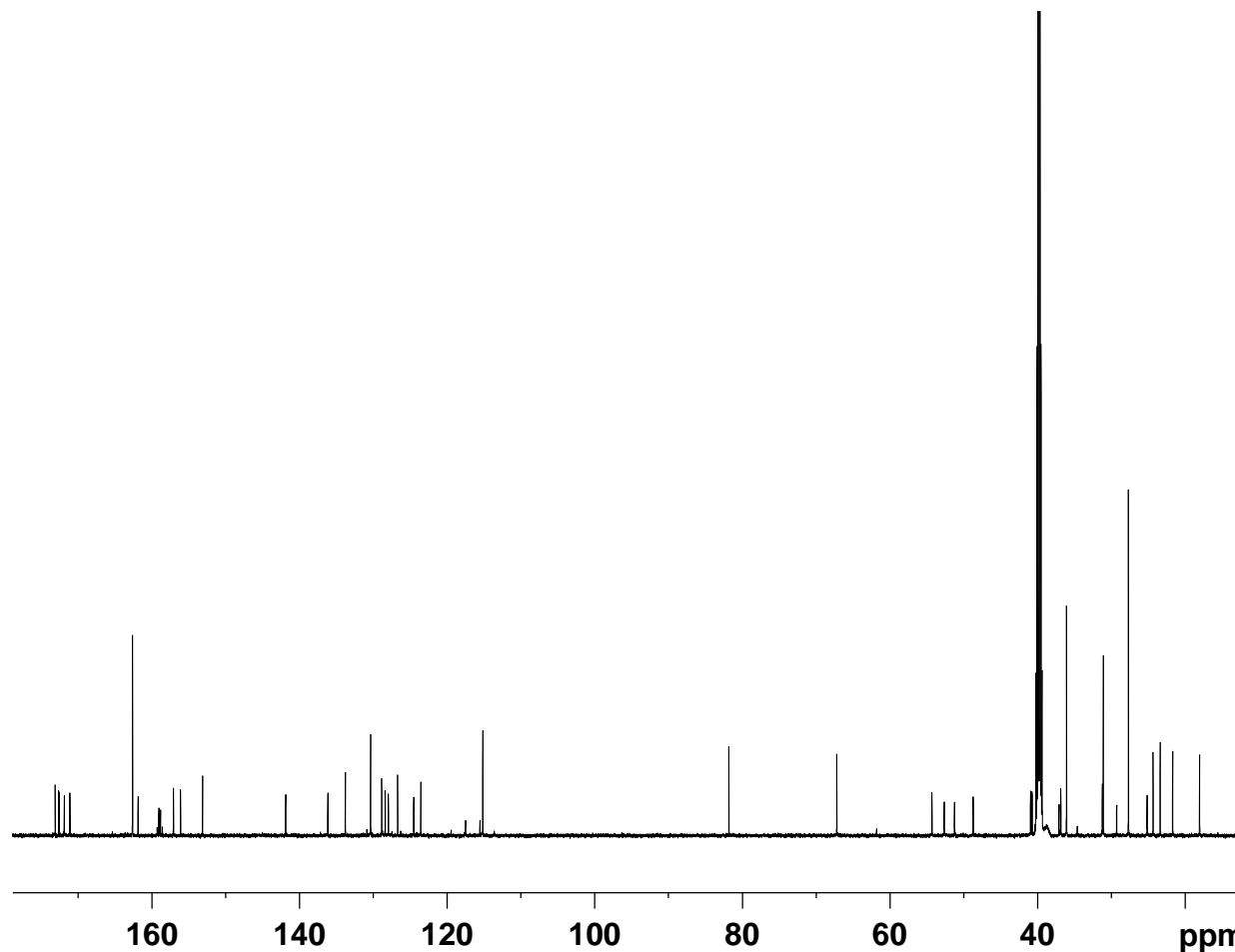
F2 - Acquisition Parameters
Date_         20110926
Time          17.17
INSTRUM       av600
PROBHD        5 mm BB5
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           12376.237 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            45.3
DW            40.400 usec
DE            6.50 usec
TE            295.3 K
D1            2.0000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
NUC1           1H
P1             14.00 usec
PL1            -1.00 dB
PL1W           31.62277603 W
SF01           600.1336008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            600.1300273 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



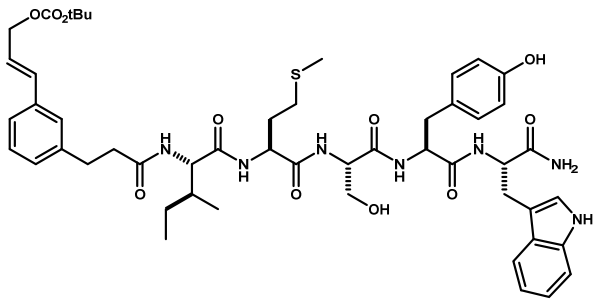
```

Current Data Parameters
NAME          KL-4-8
EXPNO         2
PROCNO        1
    
```

```

F2 - Processing parameters
SI            65536
SF            150.9028319 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

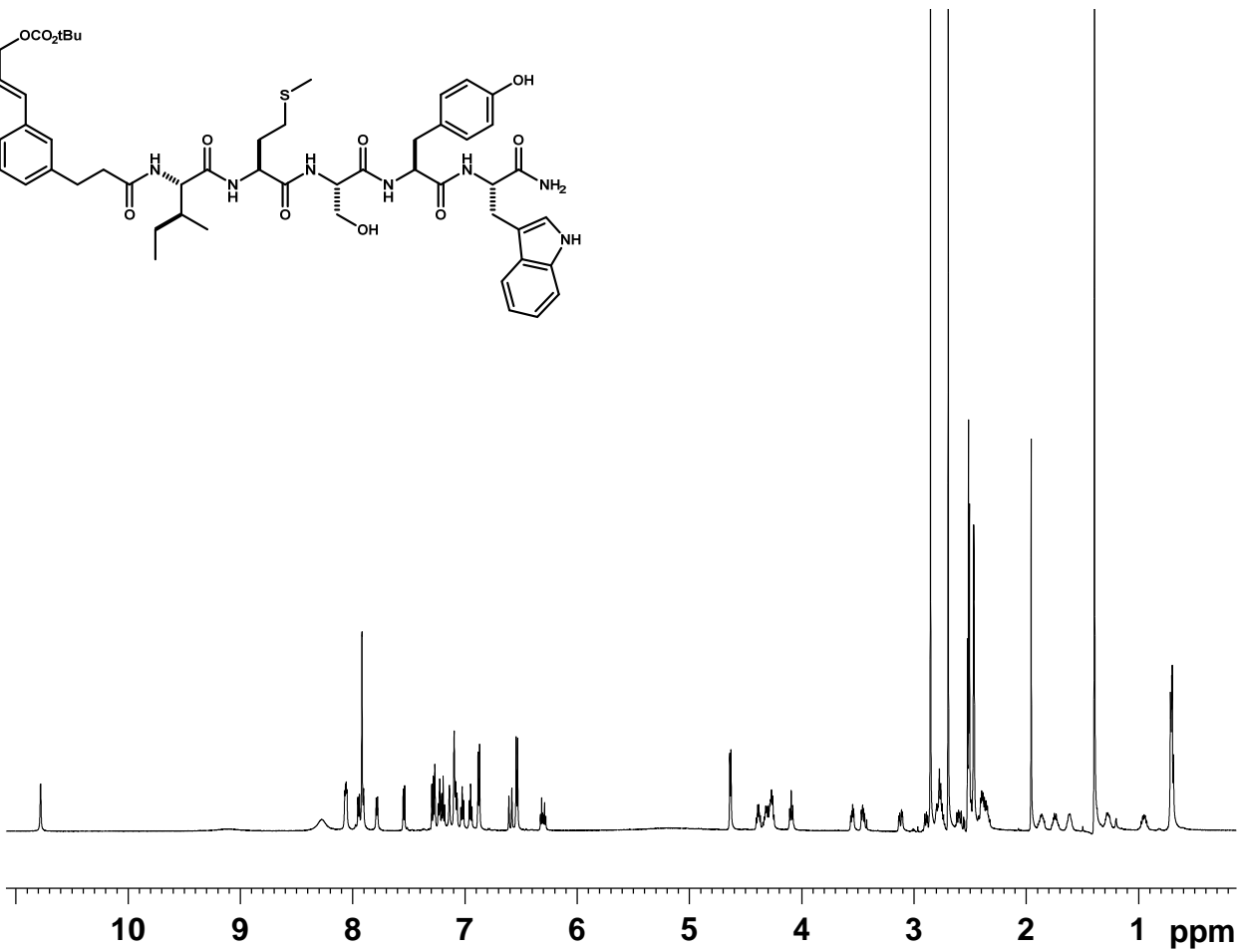
Acyclic-Ile-Met-Ser-Tyr-Trp (S15):



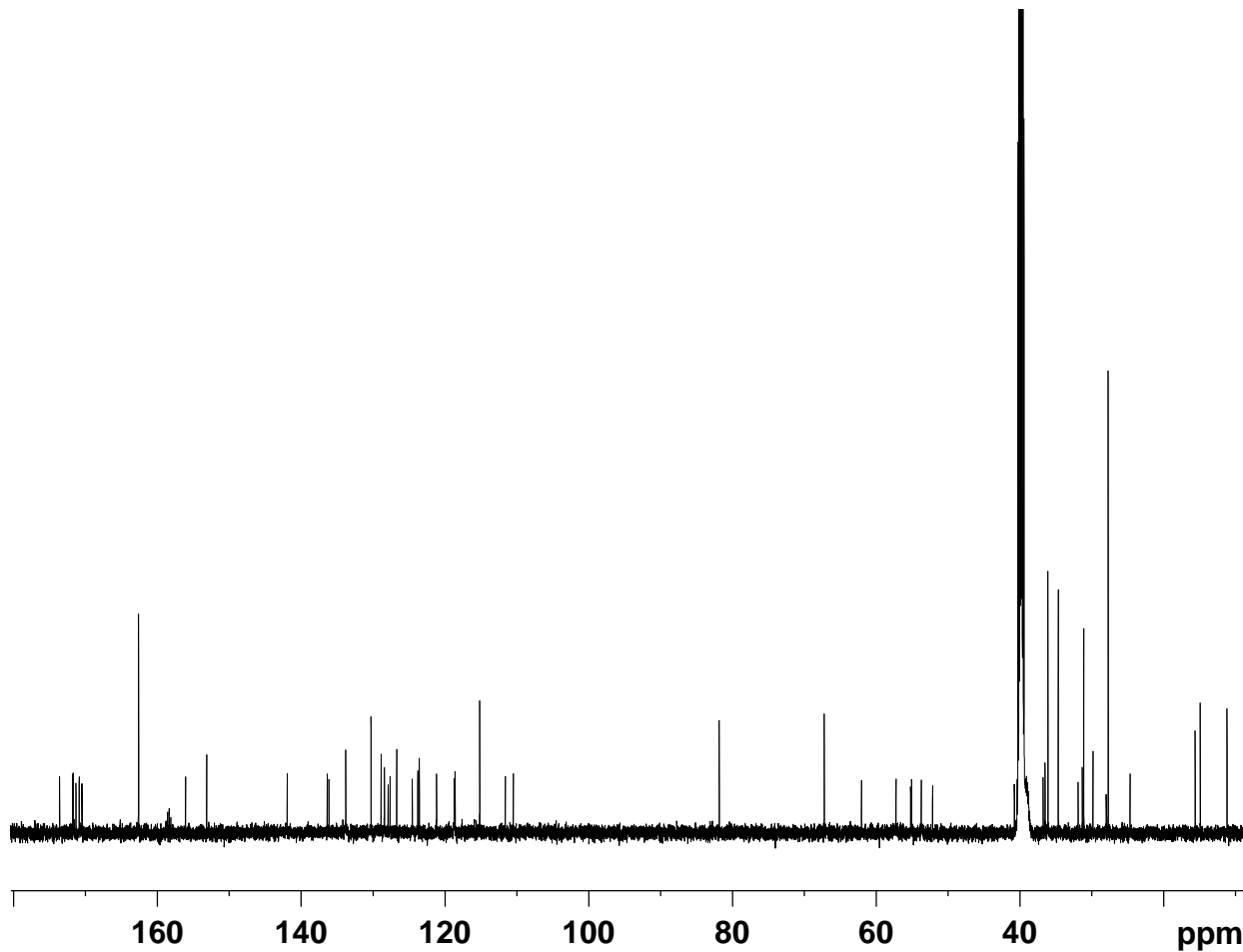
Current Data Parameters
 NAME KL-III-289
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110829
 Time 14.51
 INSTRUM av600
 PROBHD 5 mm BB5
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 12376.237 Hz
 FIDRES 0.188846 Hz
 AQ 2.6476543 sec
 RG 128
 DW 40.400 usec
 DE 6.50 usec
 TE 294.5 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -1.00 dB
 PL1W 31.62277603 W
 SFO1 600.1336008 MHz

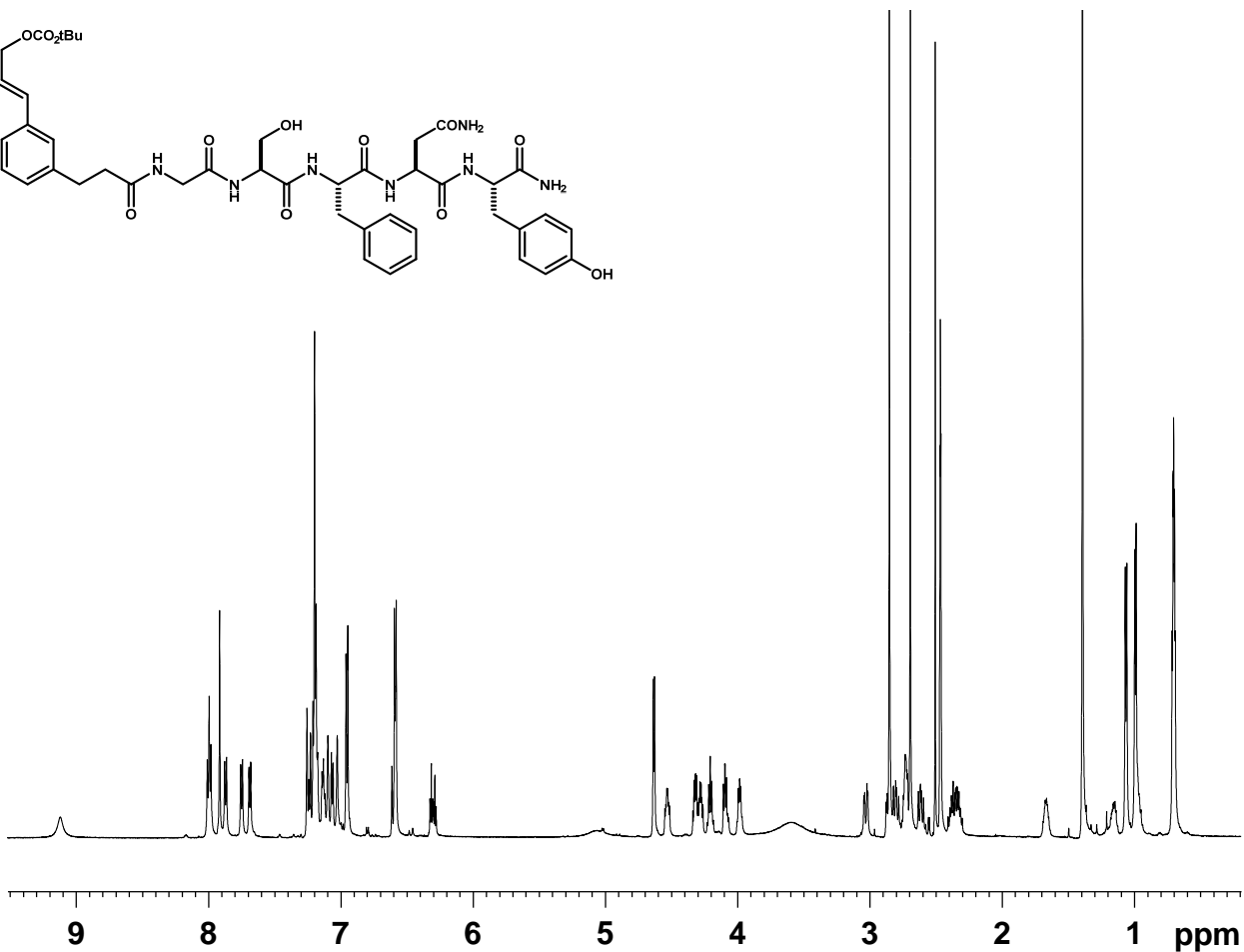
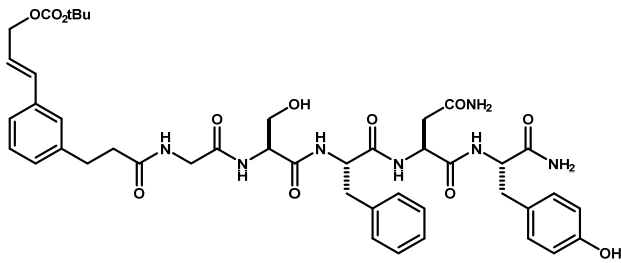
F2 - Processing parameters
 SI 65536
 SF 600.1300273 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-III-289
 EXPNO 2
 PROCNO 1
 F2 - Processing parameters
 SI 65536
 SF 150.9028319 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Acyclic-Ala-Phe-Thr-Ile-Tyr (S16):



```

Current Data Parameters
NAME          KL-III-279
EXPNO         1
PROCNO        1

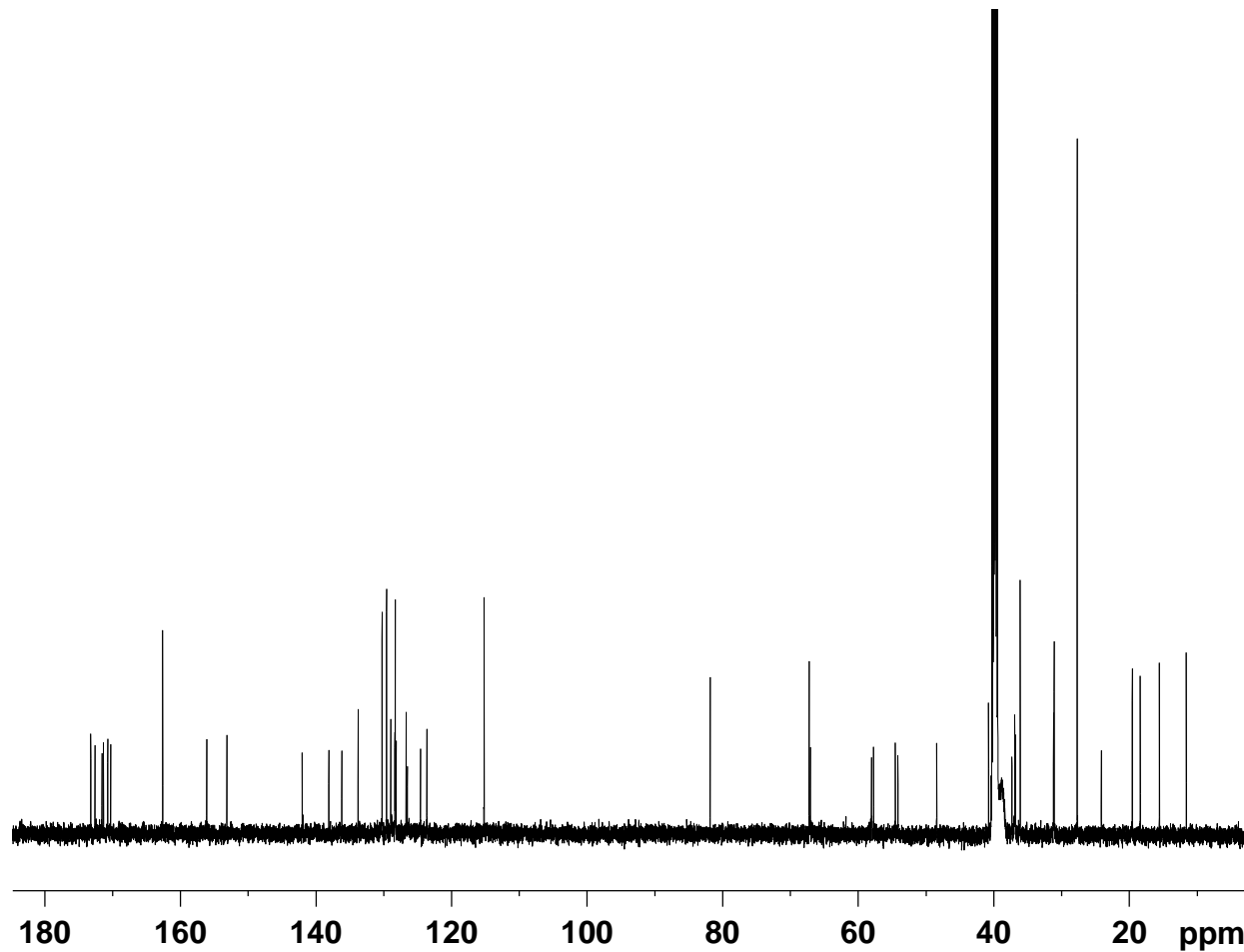
F2 - Acquisition Parameters
Date_         20110829
Time          16.16
INSTRUM       av600
PROBHD        5 mm BB5
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           12376.237 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            114
DW            40.400 usec
DE            6.50 usec
TE            294.2 K
D1            2.0000000 sec
D10           1
    
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.00 usec
PL1           -1.00 dB
PL1W          31.62277603 W
SF01          600.1336008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            600.1300273 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



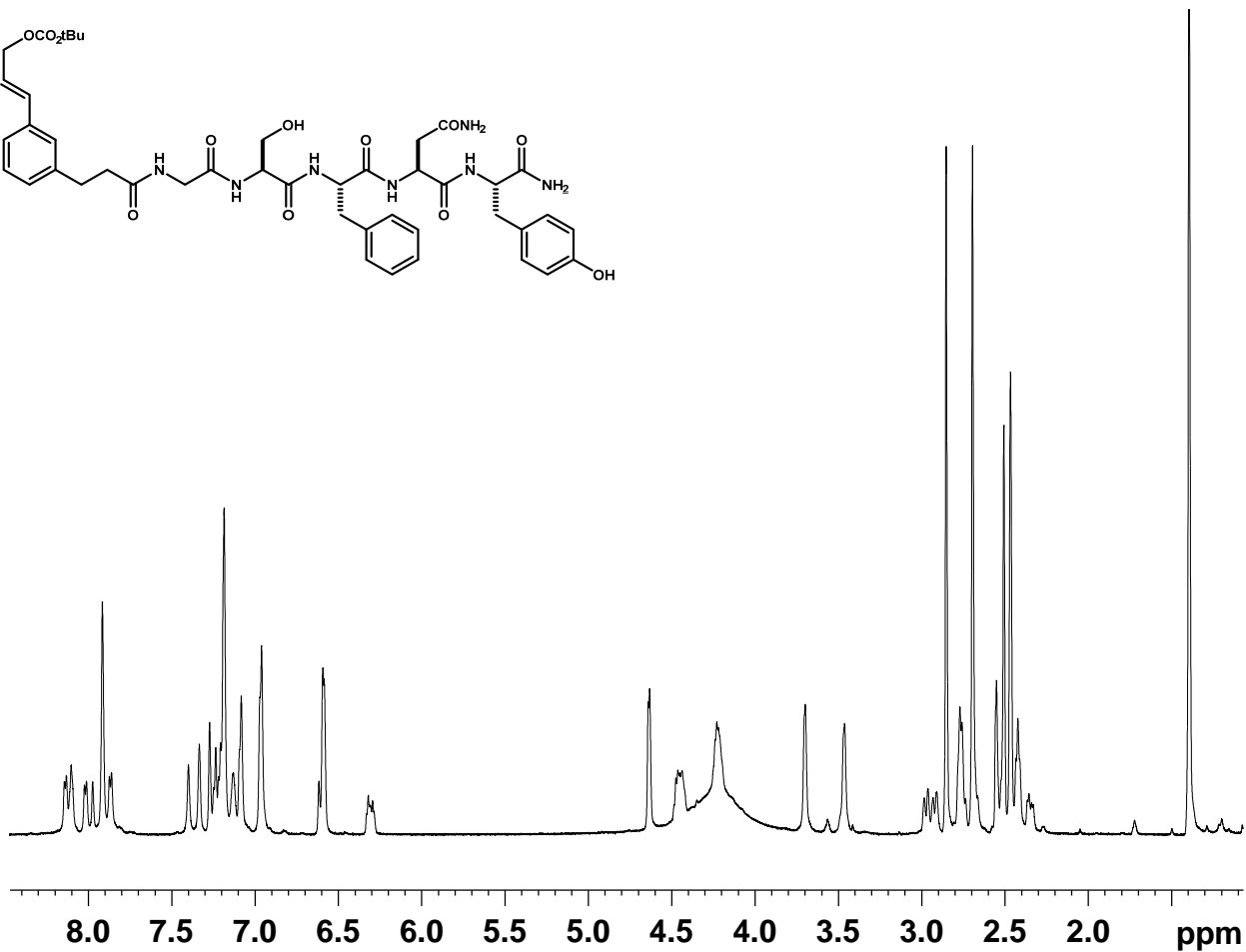
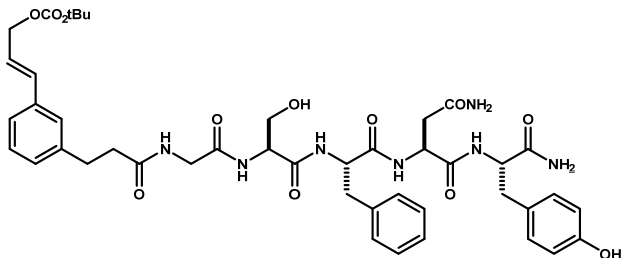
```

Current Data Parameters
NAME          KL-III-279
EXPNO         2
PROCNO        1
    
```

```

F2 - Processing parameters
SI            65536
SF            150.9028319 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```


Acyclic-Gly-Ser-Phe-Asn-Tyr (S17):

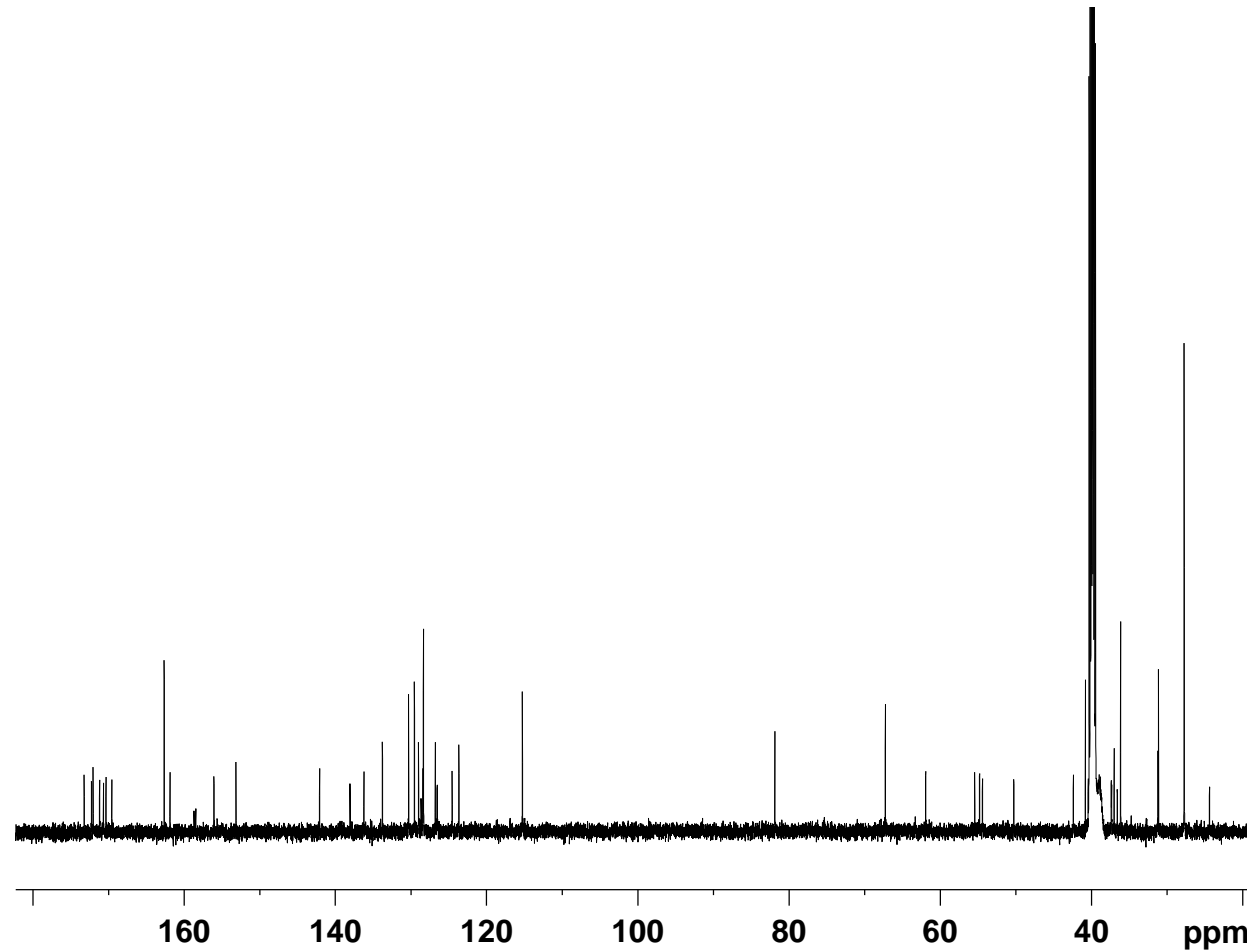


Current Data Parameters
 NAME KL-III-278
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110830
 Time 16.05
 INSTRUM av600
 PROBHD 5 mm BB5
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 12376.237 Hz
 FIDRES 0.188846 Hz
 AQ 2.6476543 sec
 RG 128
 DW 40.400 usec
 DE 6.50 usec
 TE 294.7 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -1.00 dB
 PL1W 31.62277603 W
 SFO1 600.1336008 MHz

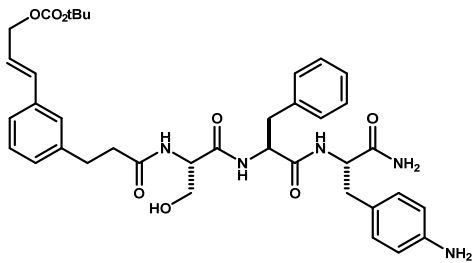
F2 - Processing parameters
 SI 65536
 SF 600.1300273 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-III-278
 EXPNO 2
 PROCNO 1

F2 - Processing parameters
 SI 65536
 SF 150.9028319 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

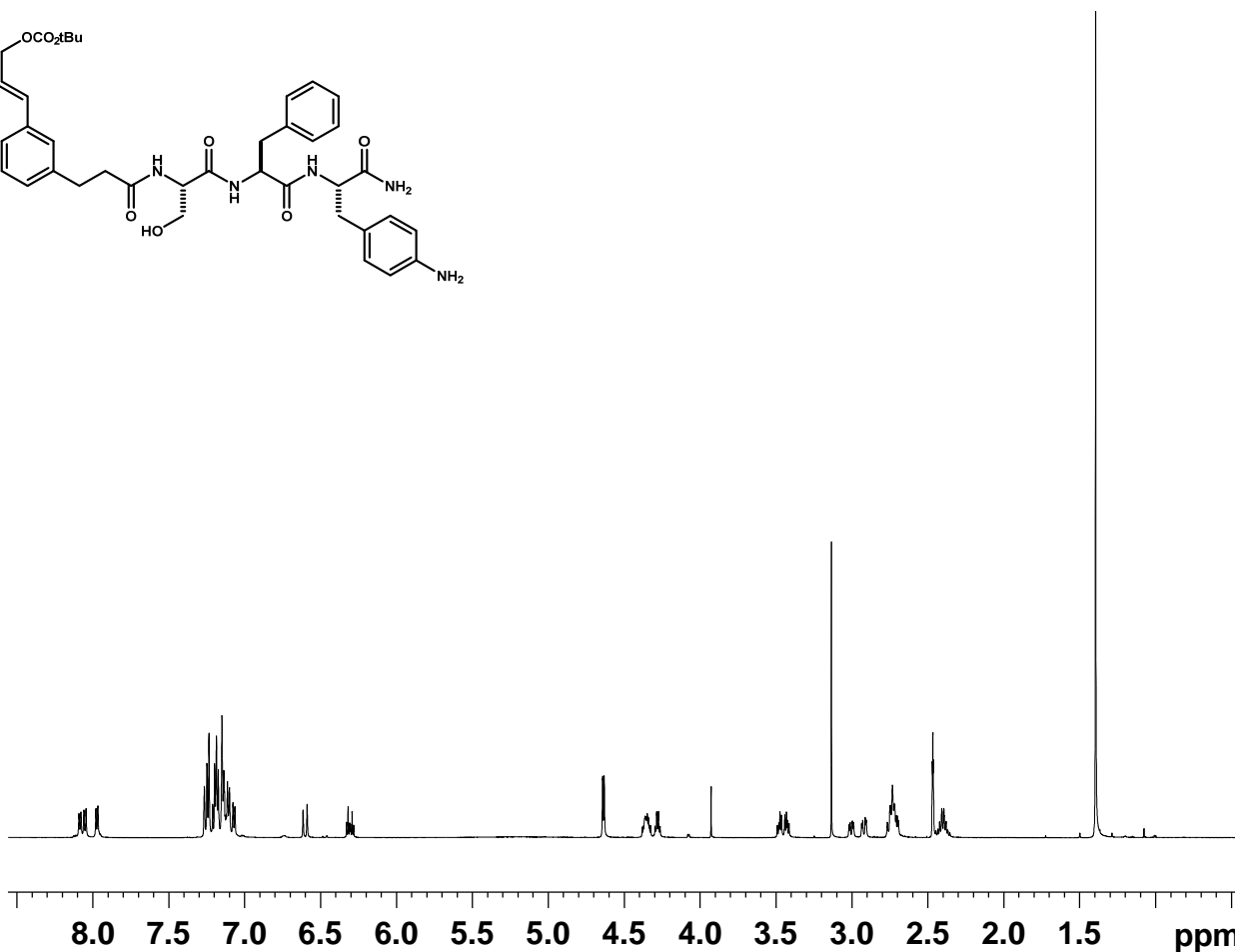
Acyclic-Ser-Phe-Phe(4-NH₂) (S18):



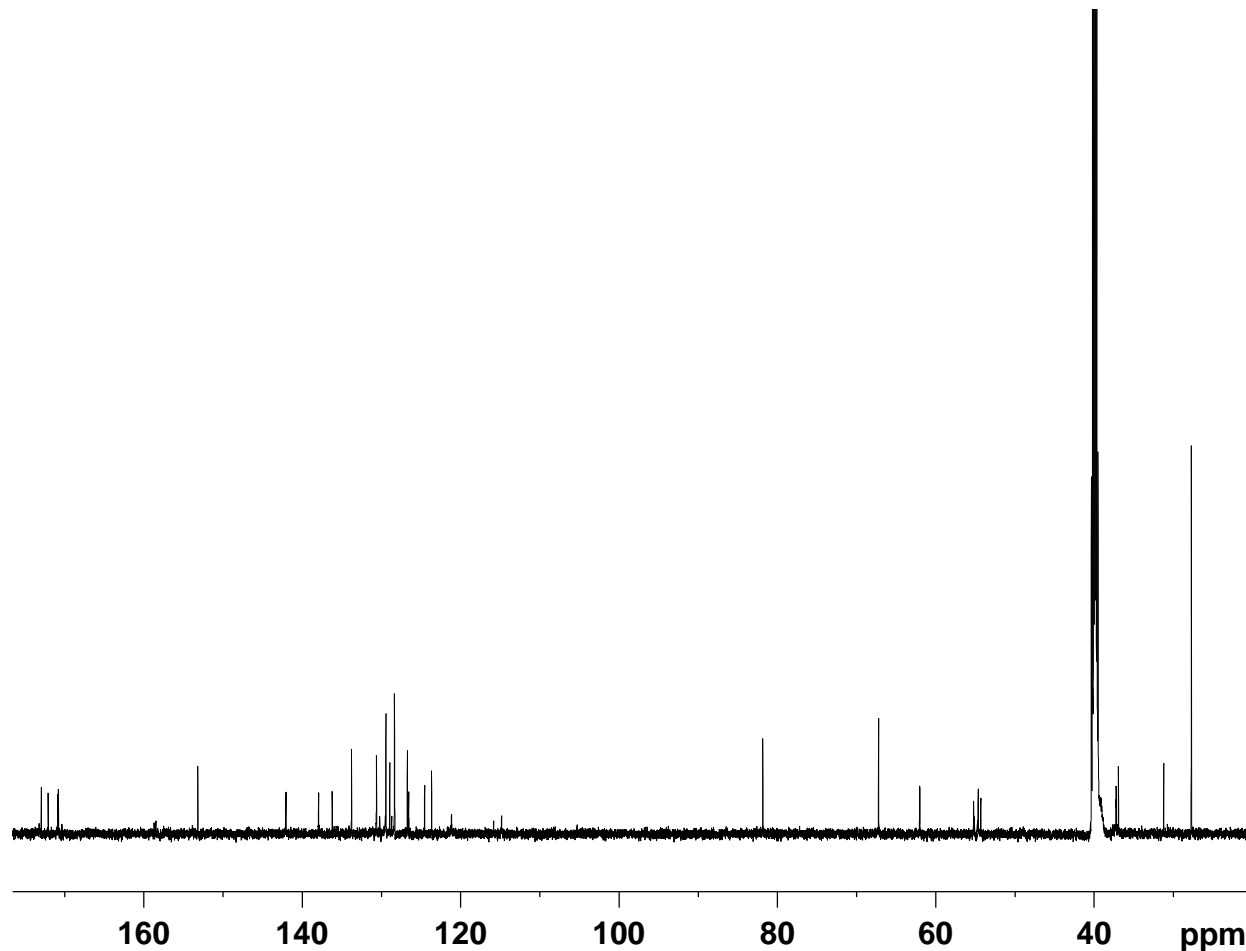
Current Data Parameters
 NAME KL-4-62_reprep
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20120125
 Time 19.30
 INSTRUM av600
 PROBHD 5 mm BB5
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 12376.237 Hz
 FIDRES 0.188846 Hz
 AQ 2.6476543 sec
 RG 161.3
 DW 40.400 usec
 DE 6.50 usec
 TE 295.2 K
 D1 2.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 8.60 usec
 PL1 -2.00 dB
 PL1W 39.81071854 W
 SFO1 600.1336008 MHz

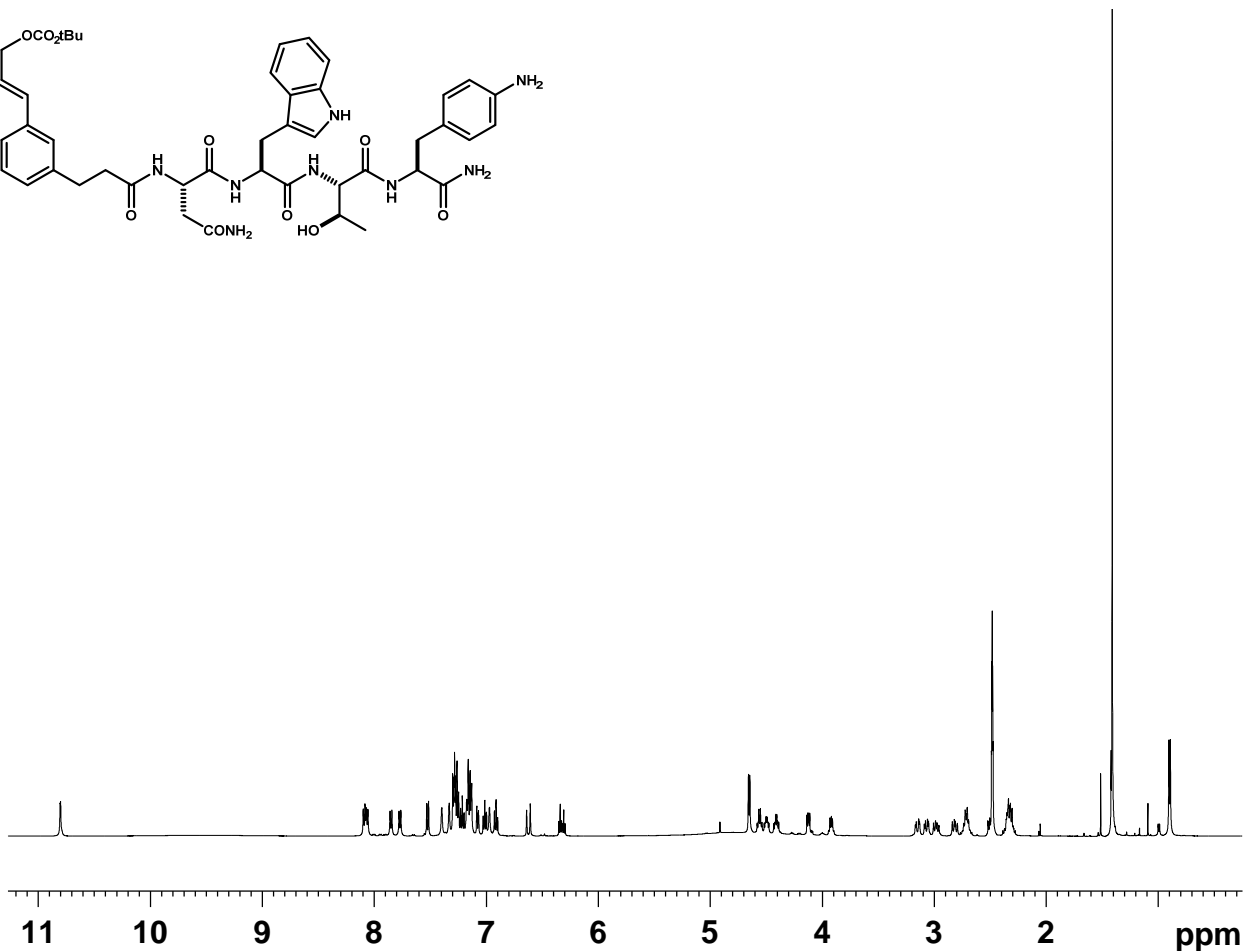
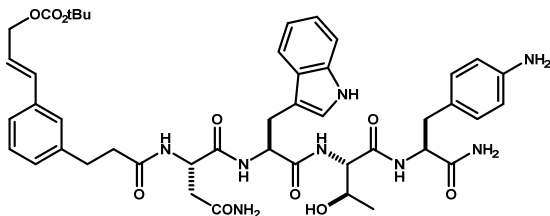
F2 - Processing parameters
 SI 65536
 SF 600.1300273 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-4-62
 EXPNO 2
 PROCNO 1
 F2 - Processing parameters
 SI 65536
 SF 150.9028319 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Acyclic-Asn-Trp-Thr-Phe(4-NH₂) (S19):

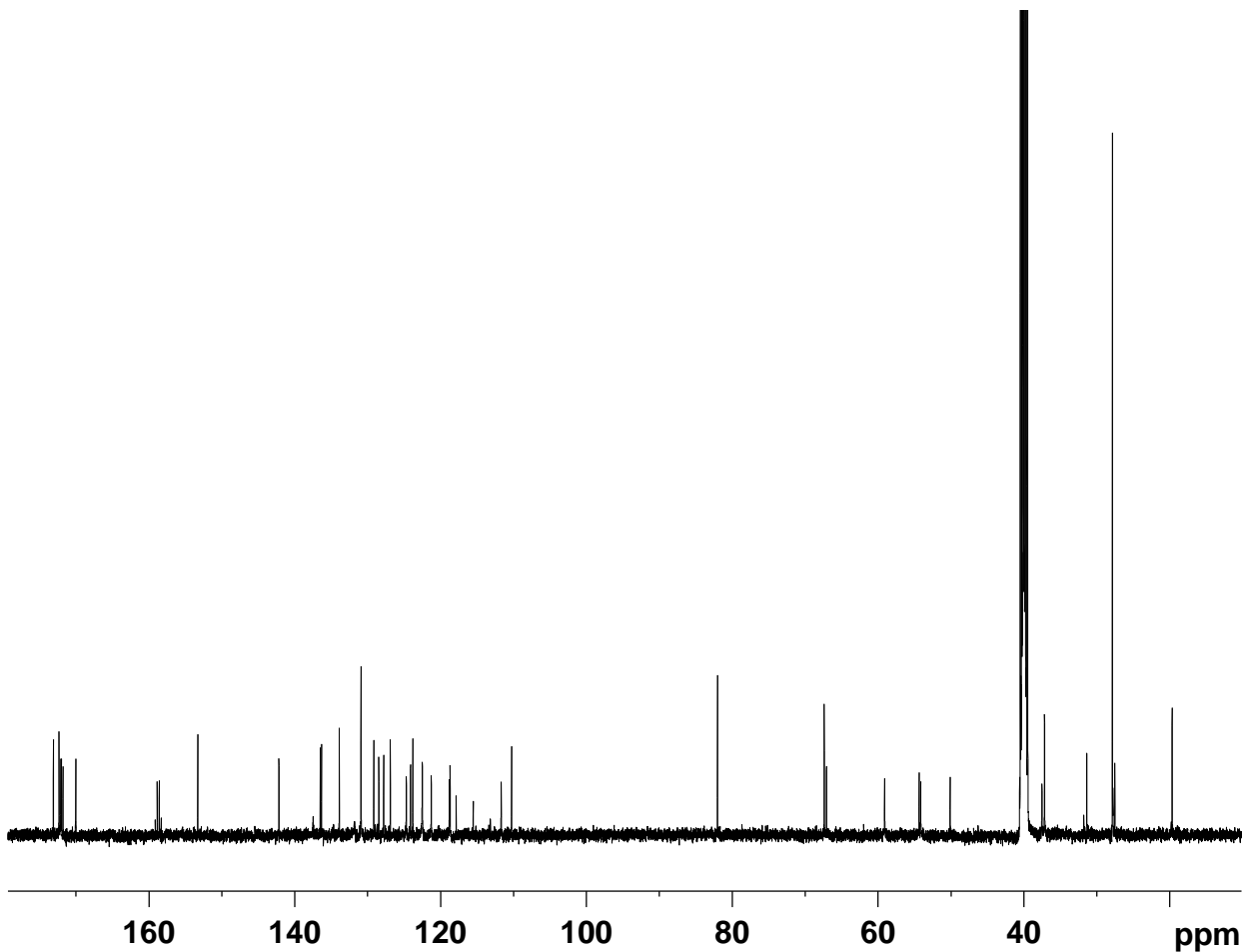


```
Current Data Parameters
NAME          KL-5-127
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20130209
Time          15.55
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            11
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1
```

```
===== CHANNEL f1 =====
SFO1          500.1330008 MHz
NUC1           1H
P1            10.00 usec
PLW1          13.5000000 W
```

```
F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



```
Current Data Parameters
NAME          KL-5-127
EXPNO         2
PROCNO        1

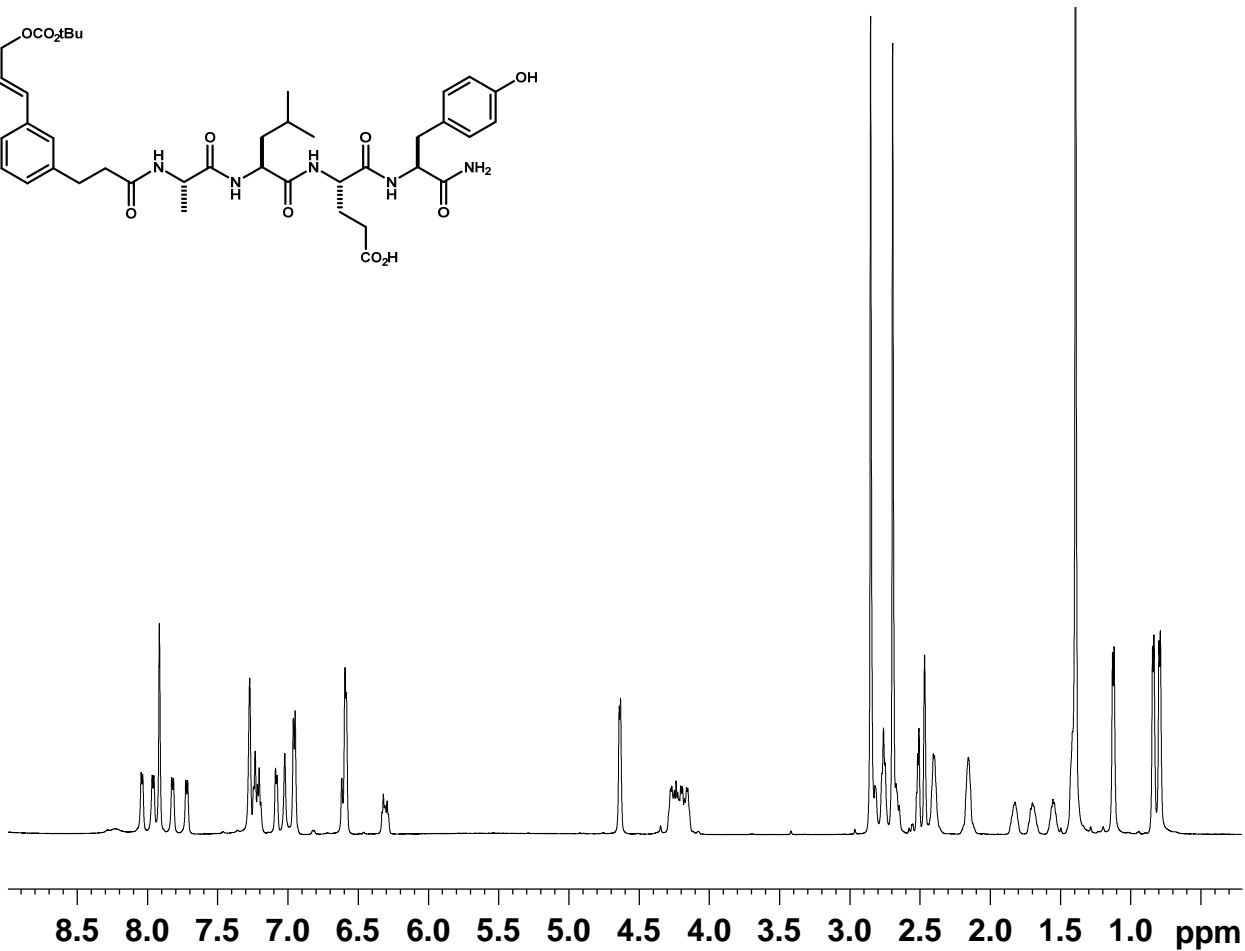
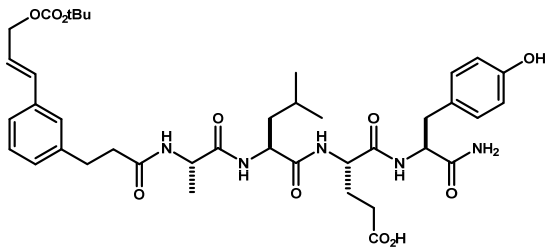
F2 - Acquisition Parameters
Date_         20130209
Time          15.58
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            66
DS            2
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG            202.91
DW            16.000 usec
DE            18.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
```

```
===== CHANNEL f1 =====
SFO1          125.7722511 MHz
NUC1           13C
P1             9.63 usec
PLW1          23.0000000 W
```

```
===== CHANNEL f2 =====
SFO2          500.1330008 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          13.5000000 W
PLW12         0.21094000 W
PLW13         0.13500001 W
```

```
F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

Acyclic-Ala-Leu-Glu-Tyr (15):



```

Current Data Parameters
NAME          KL-III-283
EXPNO         1
PROCNO        1

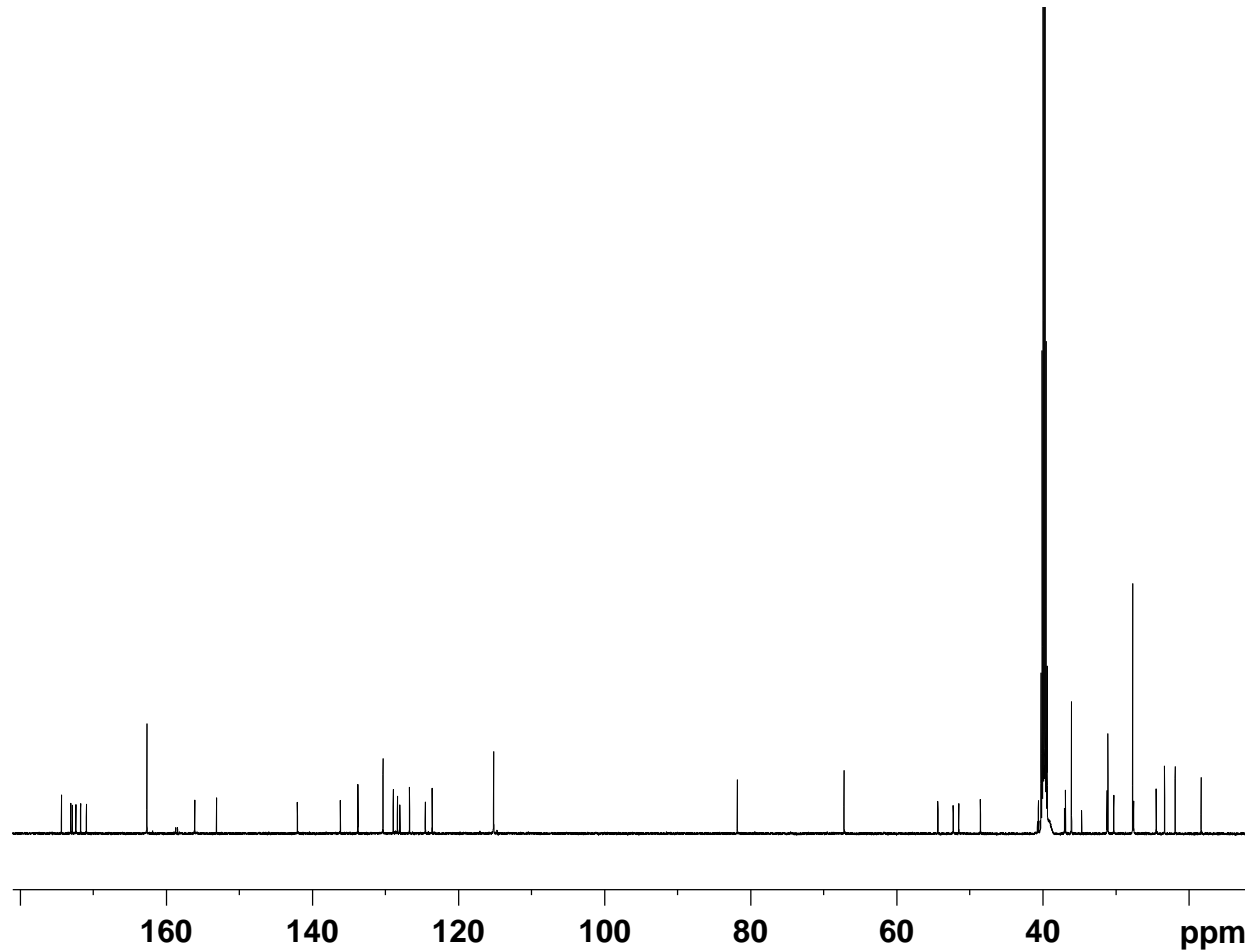
F2 - Acquisition Parameters
Date_         20110830
Time          17.22
INSTRUM       av600
PROBHD        5 mm BB5
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           12376.237 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            71.8
DW            40.400 usec
DE            6.50 usec
TE            294.7 K
D1            2.0000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            14.00 usec
PL1           -1.00 dB
PL1W          31.62277603 W
SFO1          600.1336008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            600.1300273 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

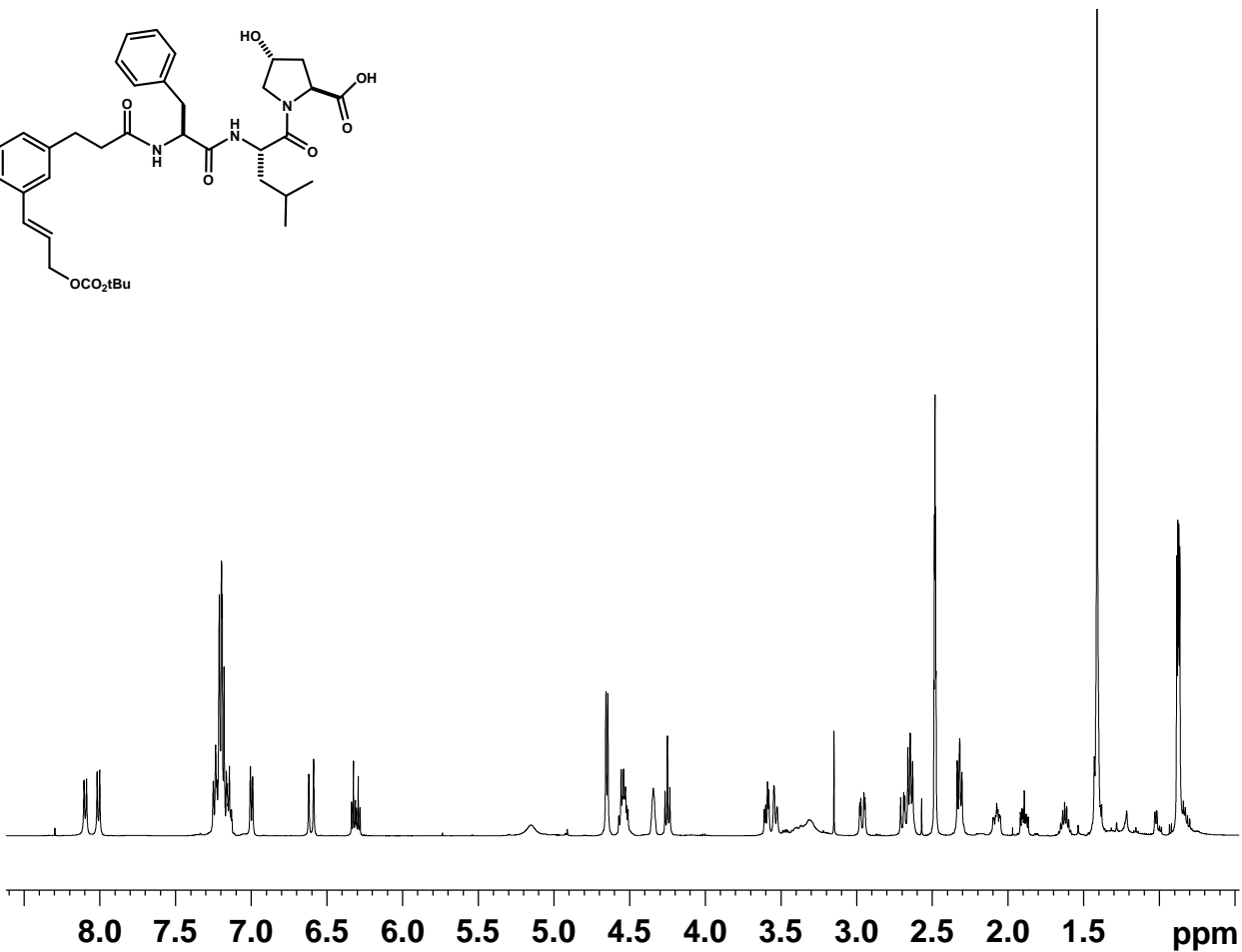
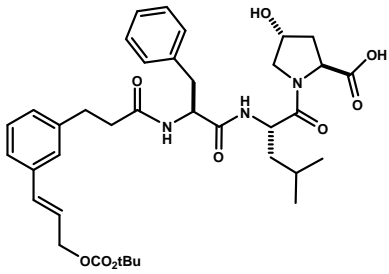


```

Current Data Parameters
NAME          KL-III-283
EXPNO         2
PROCNO        1

F2 - Processing parameters
SI            65536
SF            150.9028319 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

Acyclic-Phe-Leu-Hyp (S21):

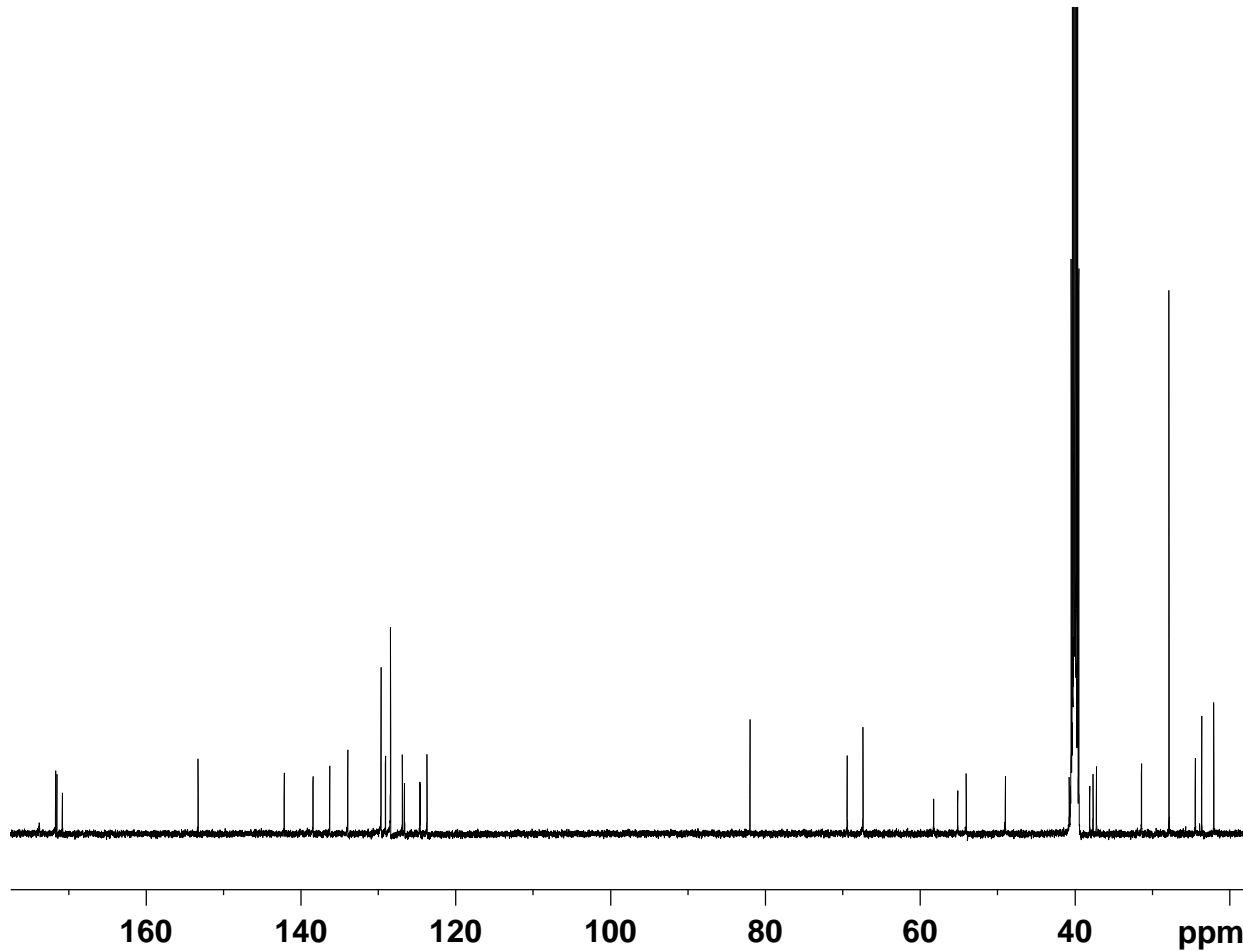


Current Data Parameters
NAME KL-5-11
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120821
Time 17.09
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 129.78
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PLW1 13.5000000 W
SFO1 500.1330008 MHz

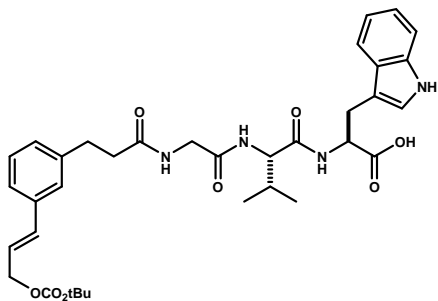
F2 - Processing parameters
SI 65536
SF 500.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME KL-5-11
EXPNO 2
PROCNO 1

F2 - Processing parameters
SI 131072
SF 125.7577892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Acyclic-Gly-Val-Trp (S22):



```

Current Data Parameters
NAME          KL-4-188
EXPNO         1
PROCNO        1

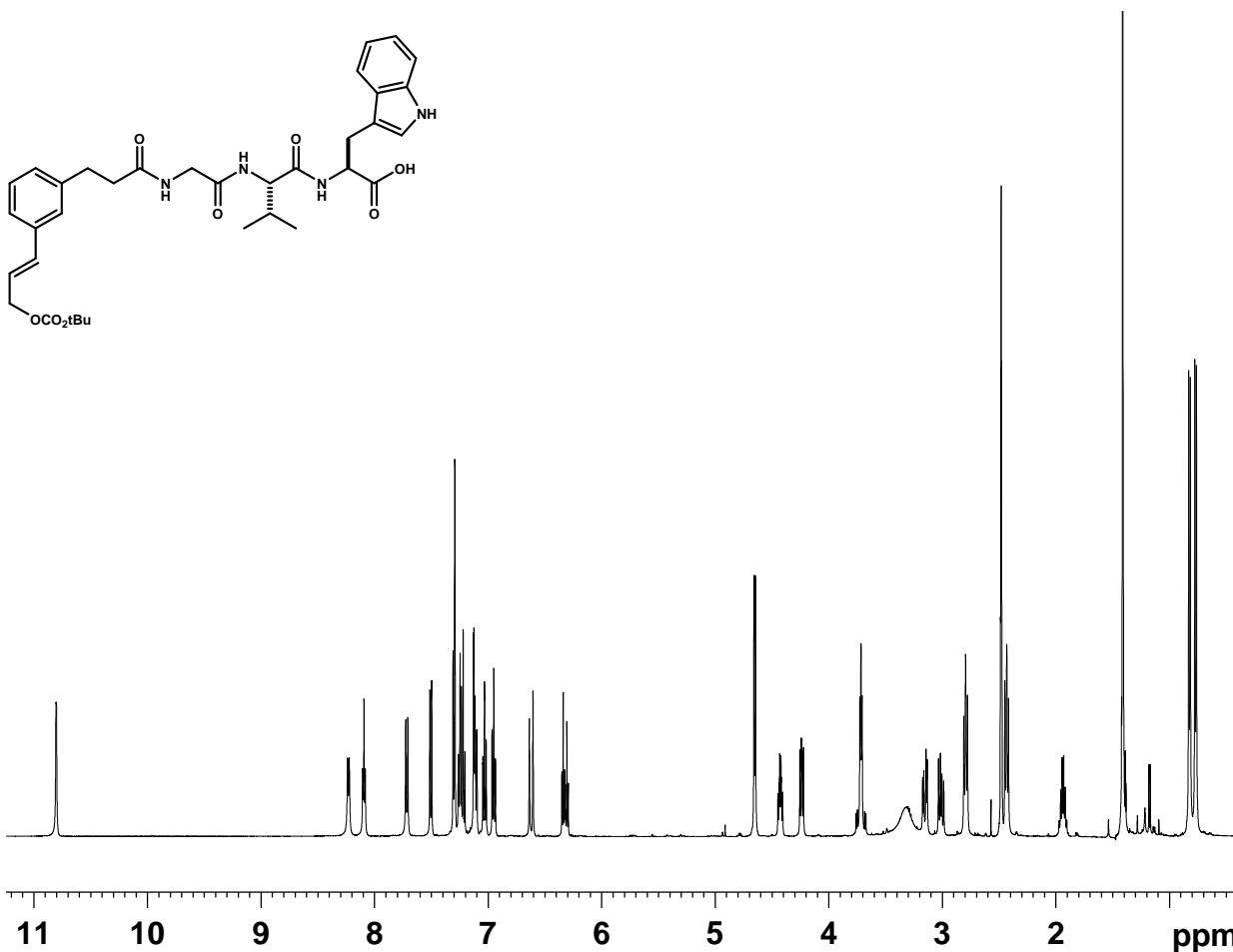
F2 - Acquisition Parameters
Date_         20120821
Time          19.01
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            145.12
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.00000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            10.00 usec
PLW1         13.50000000 W
SFO1         500.1330008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0 Hz
GB            0
PC            1.00
    
```

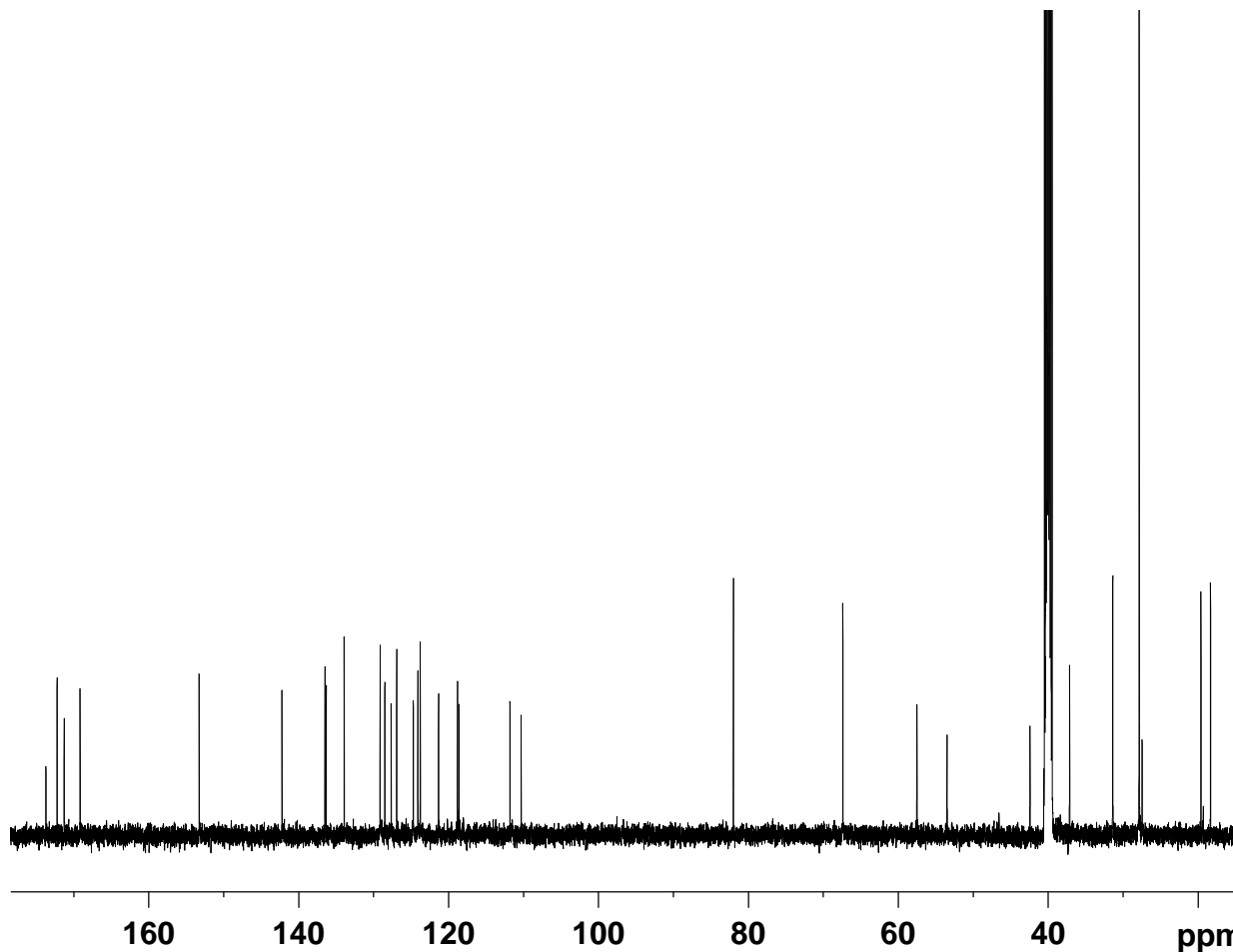


```

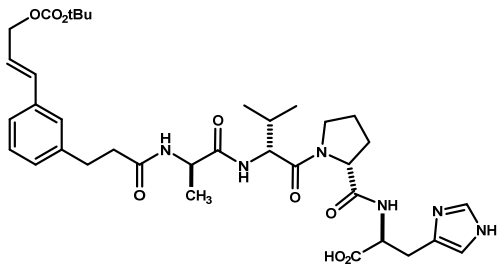
Current Data Parameters
NAME          KL-4-188
EXPNO         2
PROCNO        1
    
```

```

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

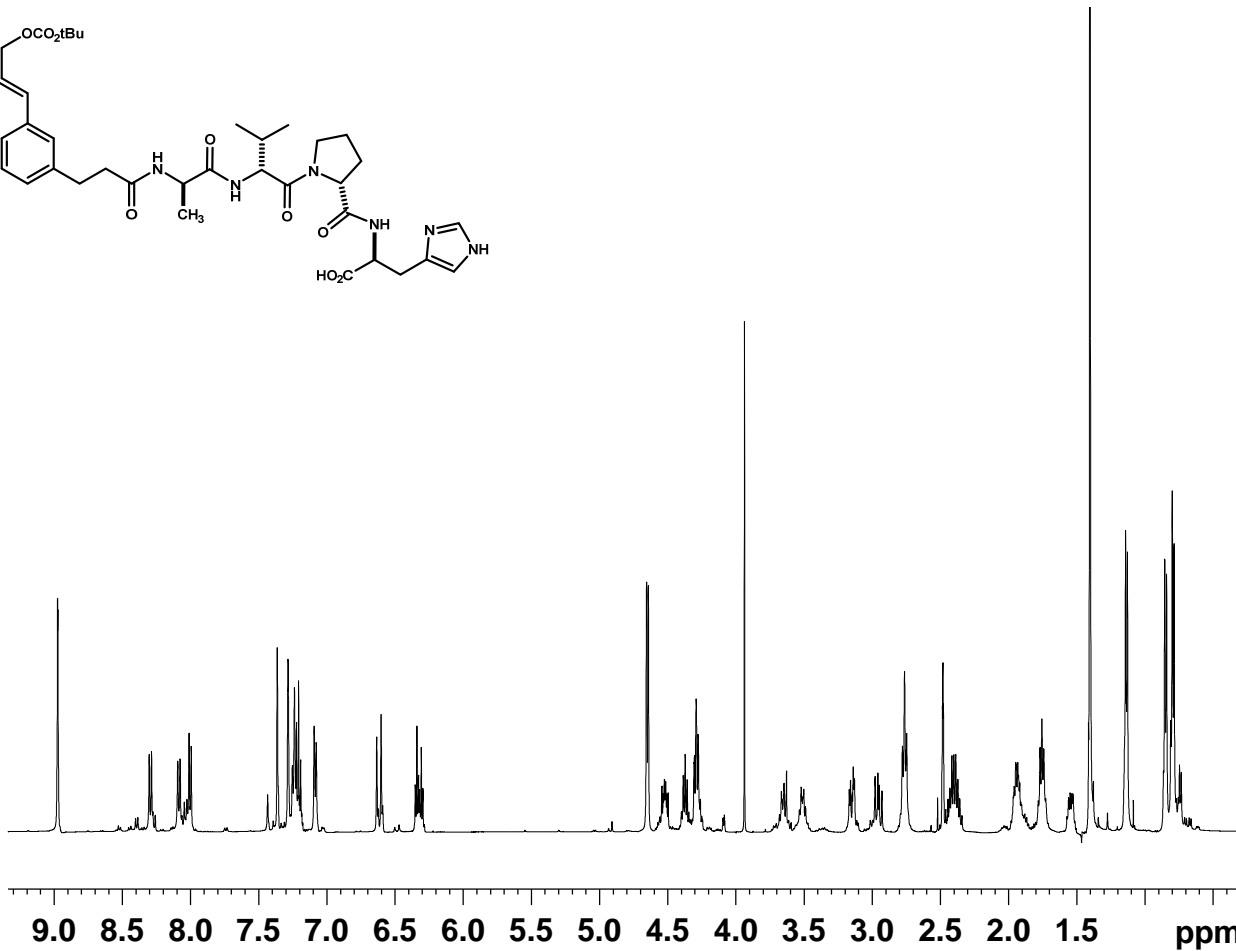


Acyclic-Ala-Val-Pro-His-OH (S23):

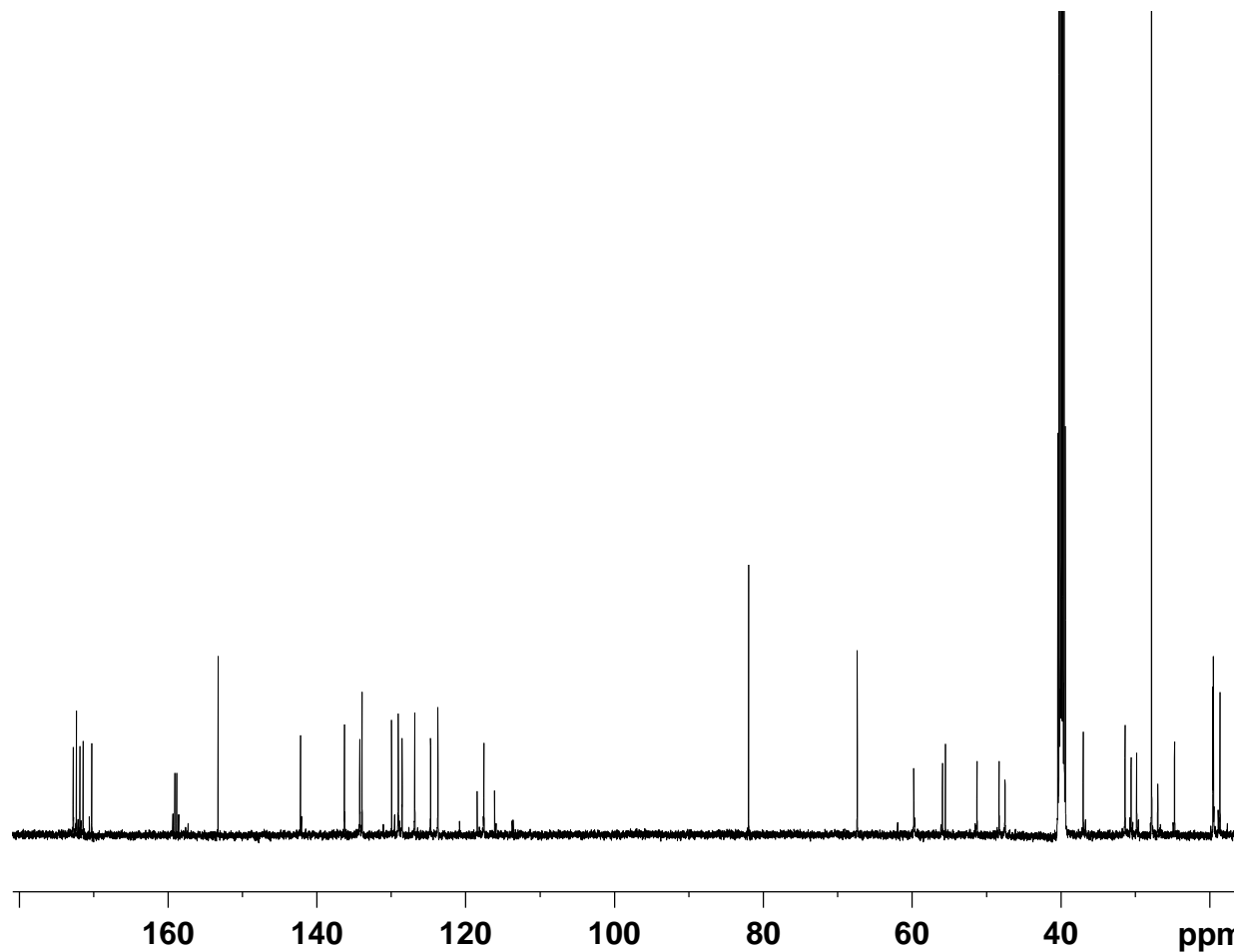


Current Data Parameters
 NAME KL-4-161
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20120329
 Time 17.31
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 11
 DW 50.000 usec
 DE 10.00 usec
 TE 296.0 K
 D1 2.00000000 sec
 TDO 1

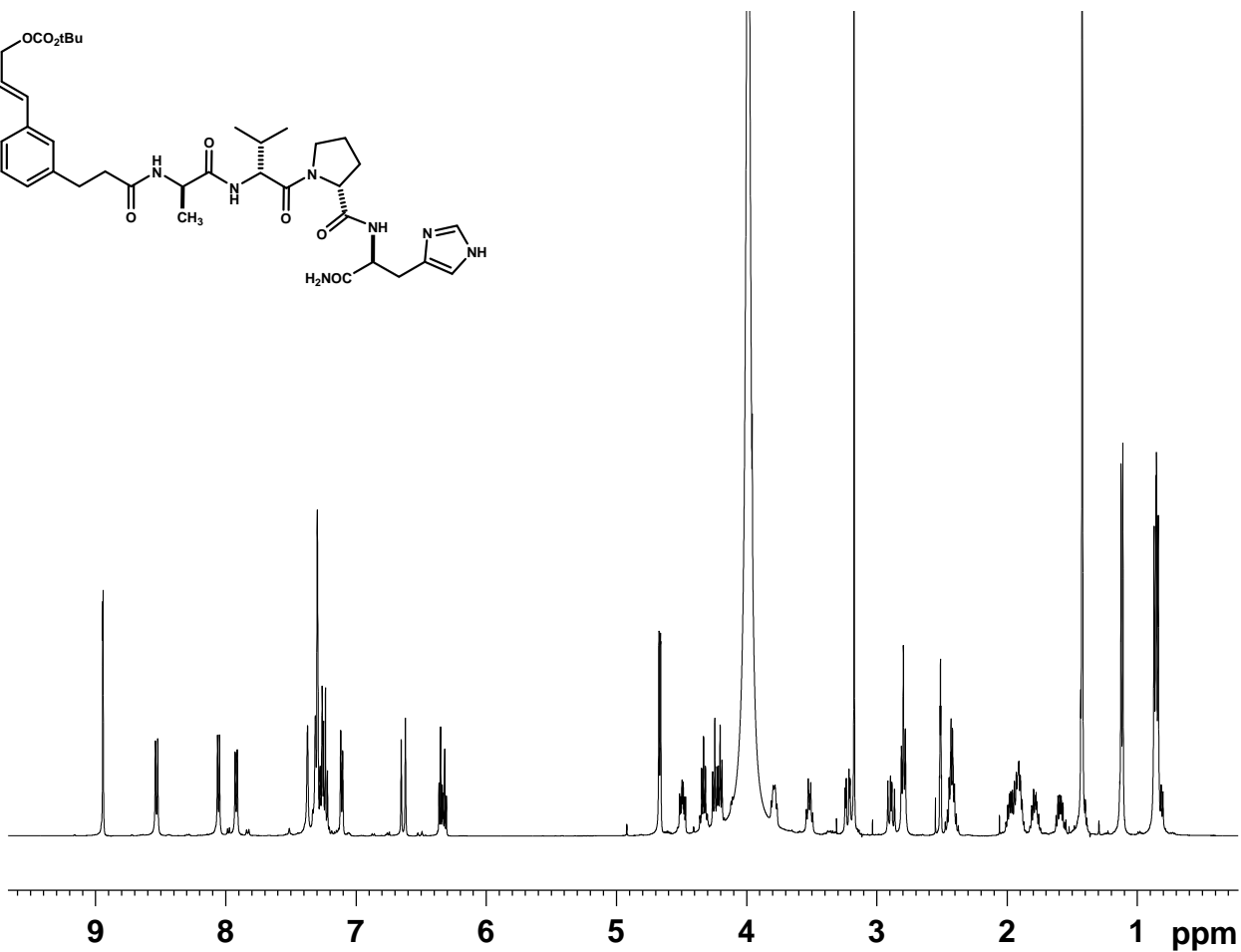
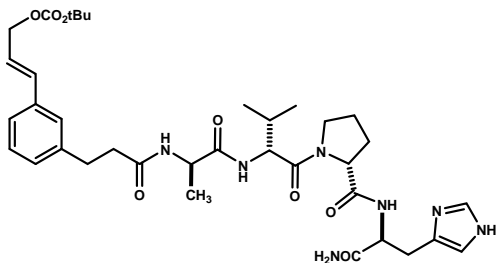
==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PLW1 13.5000000 W
 SFO1 500.1330008 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.1300146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-4-161
 EXPNO 1
 PROCNO 1
 F2 - Processing parameters
 SI 131072
 SF 125.7577892 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

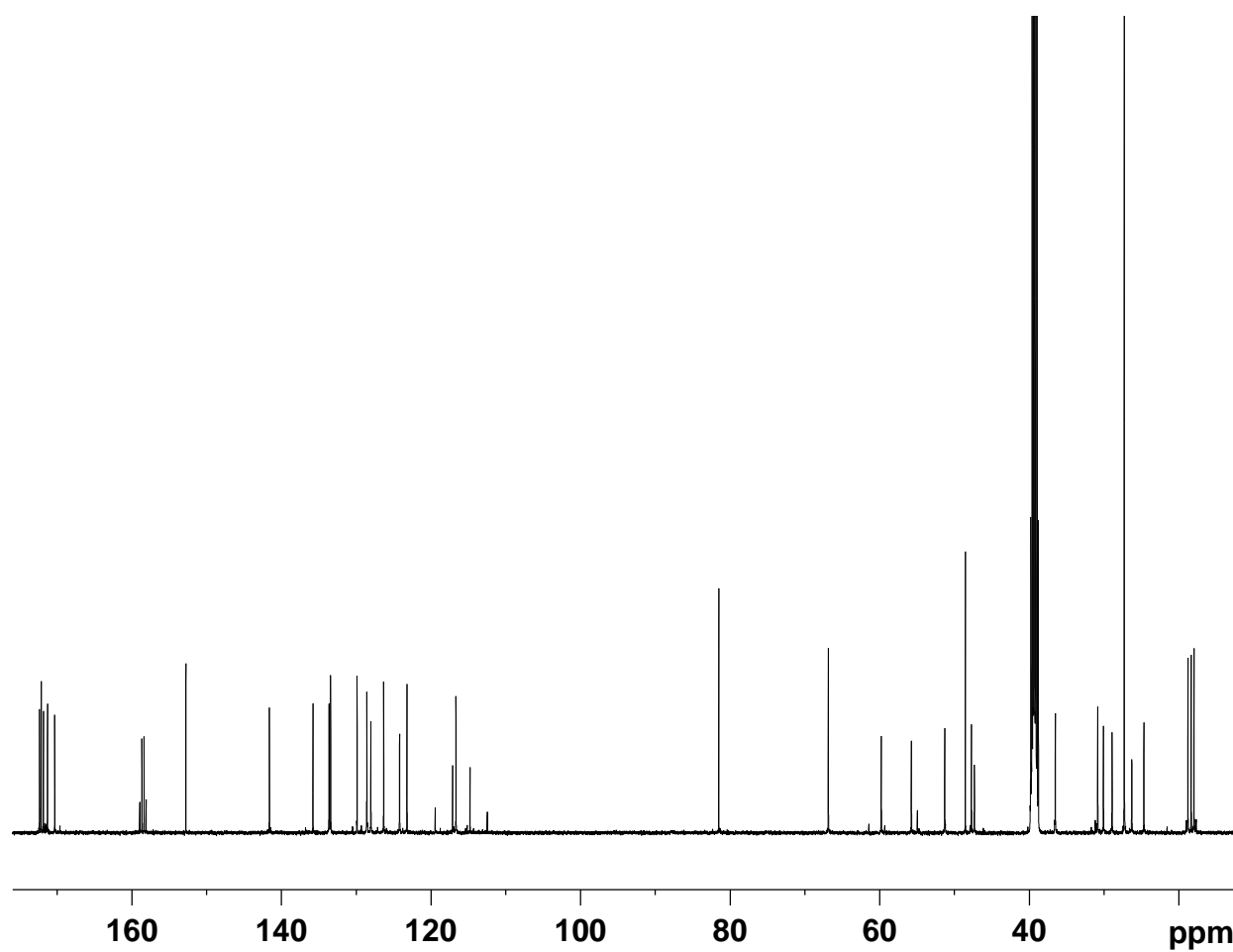


Acyclic-Ala-Val-Pro-His-NH₂ (S24):



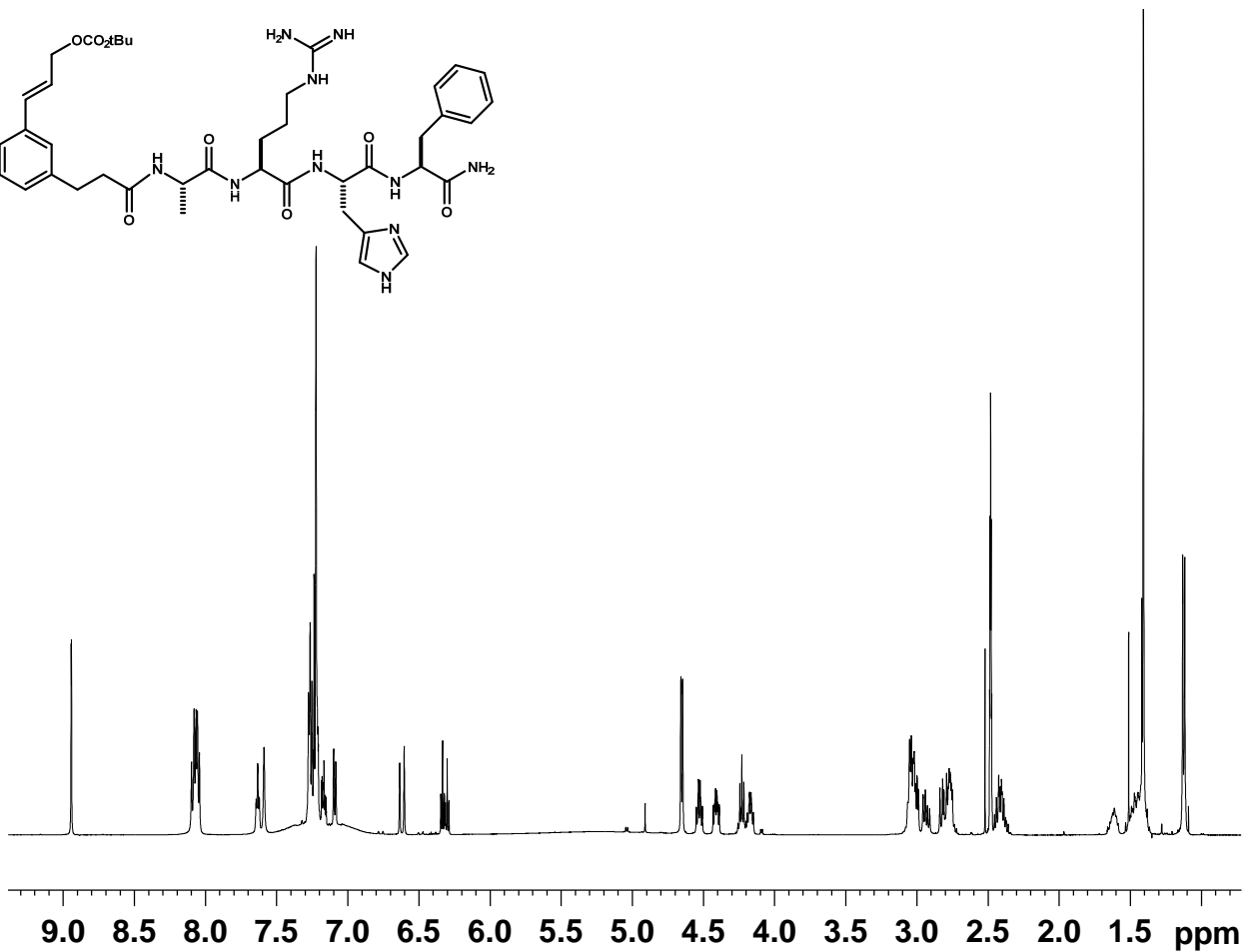
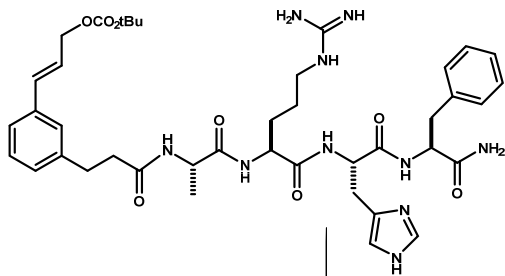
Current Data Parameters
 NAME ICON-W-B5
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20121013
 Time 13.40
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 11
 DW 50.000 usec
 DE 10.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PLW1 13.5000000 W
 SFO1 500.1330008 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME ICON-W-B5
 EXPNO 2
 PROCNO 1
 F2 - Processing parameters
 SI 131072
 SF 125.7578519 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Acyclic-Ala-Arg-His-Phe-NH₂ (S25):



```

Current Data Parameters
NAME      HIS_A5
EXPNO    10
PROCNO   1

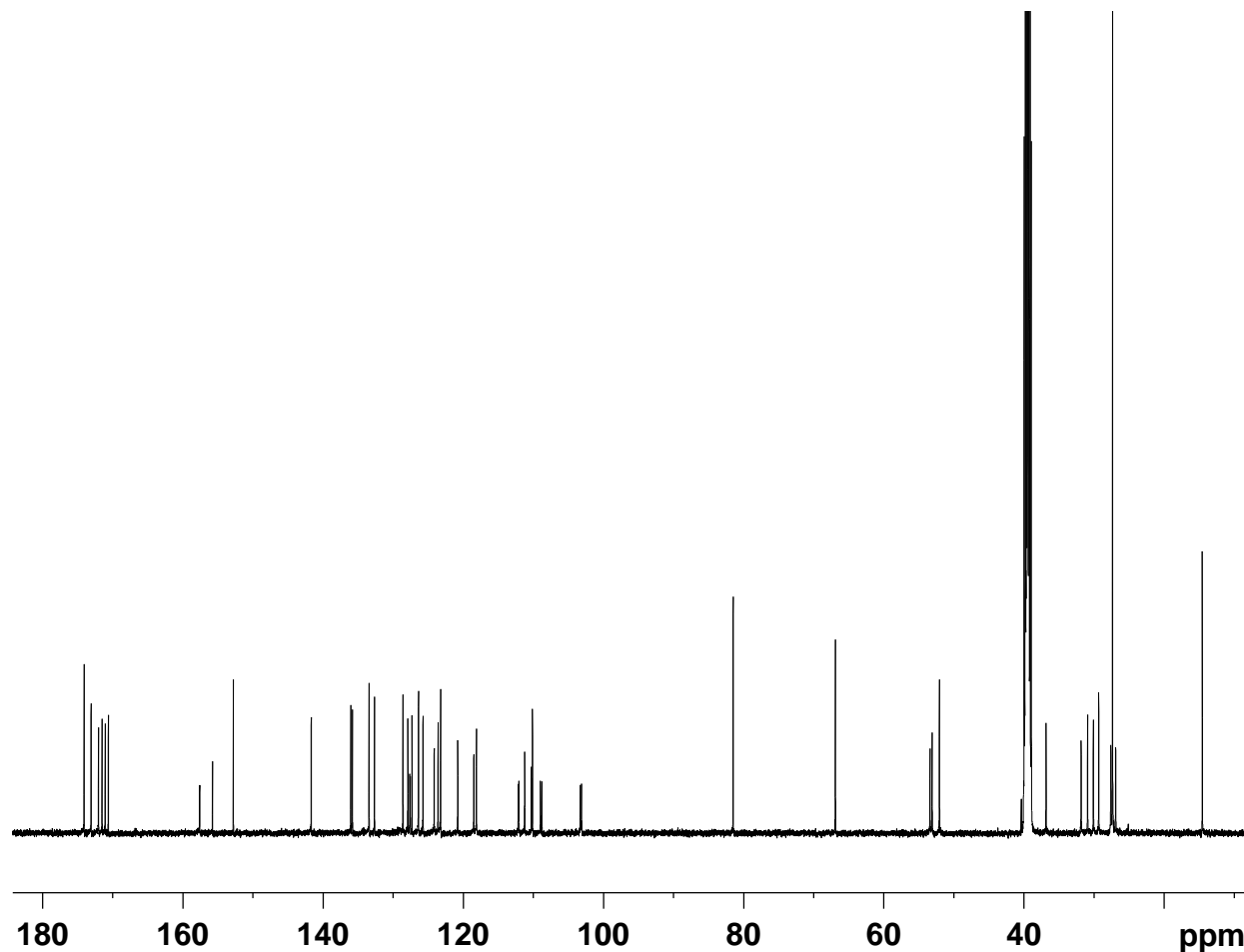
F2 - Acquisition Parameters
Date_    20121130
Time     17.23
INSTRUM av500
PROBHD   5 mm DCH 13C-1
PULPROG zg30
TD       65536
SOLVENT  DMSO
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       11
DW       50.000 usec
DE       10.00 usec
TE       298.0 K
D1       2.0000000 sec
TD0      1
    
```

```

===== CHANNEL f1 =====
SF01    500.1330008 MHz
NUC1     1H
P1       10.00 usec
PLW1    13.5000000 W
    
```

```

F2 - Processing parameters
SI       65536
SF       500.1300146 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



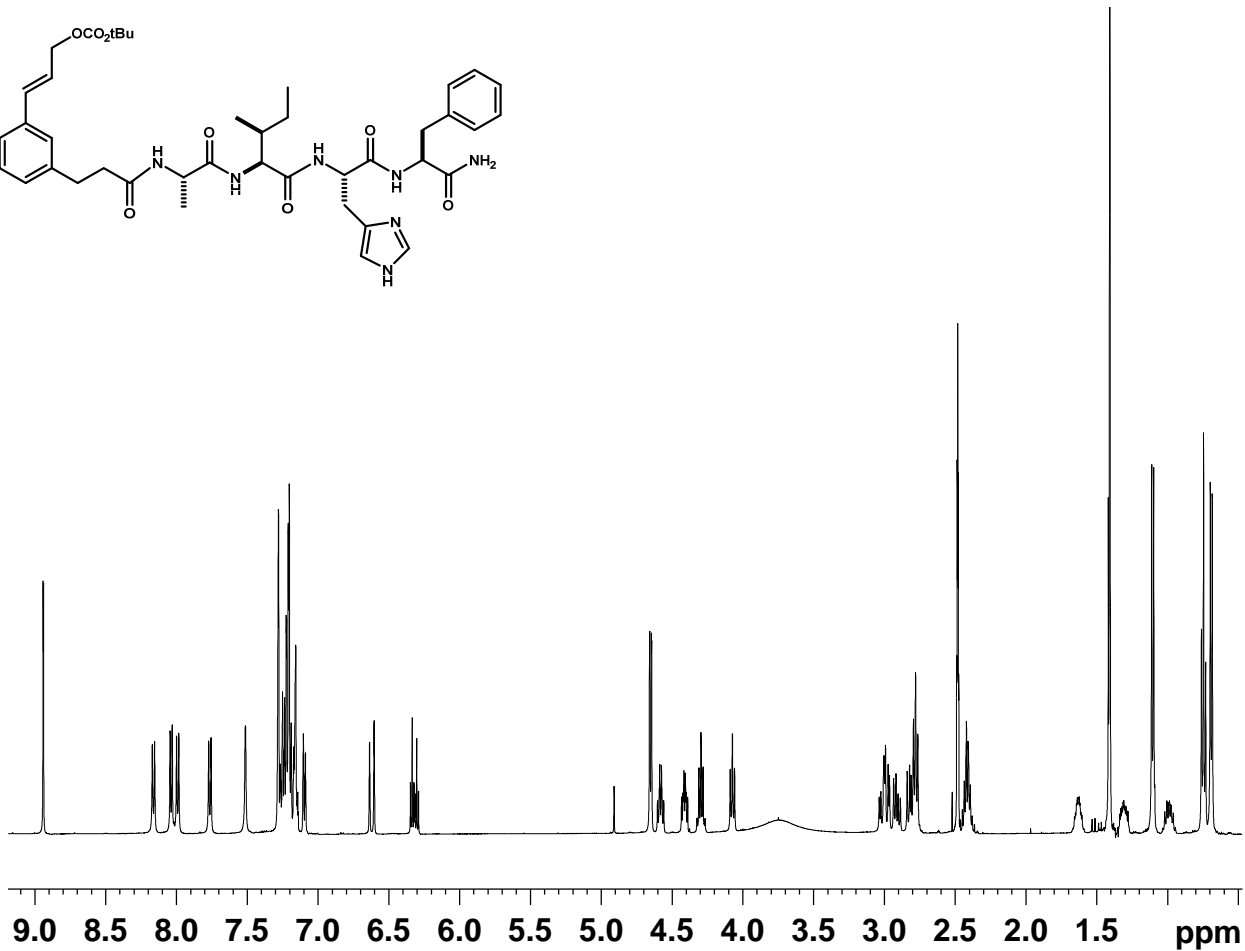
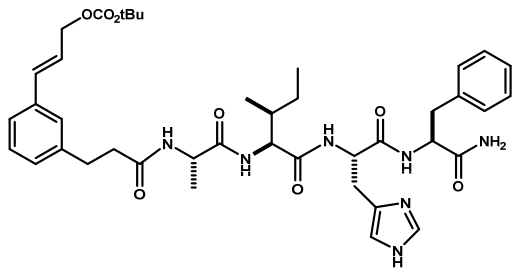
```

Current Data Parameters
NAME      ICON-W-A5
EXPNO    2
PROCNO   1
    
```

```

F2 - Processing parameters
SI       131072
SF       125.7578519 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

Acyclic-Ala-Ile-His-Phe-NH₂ (S26):



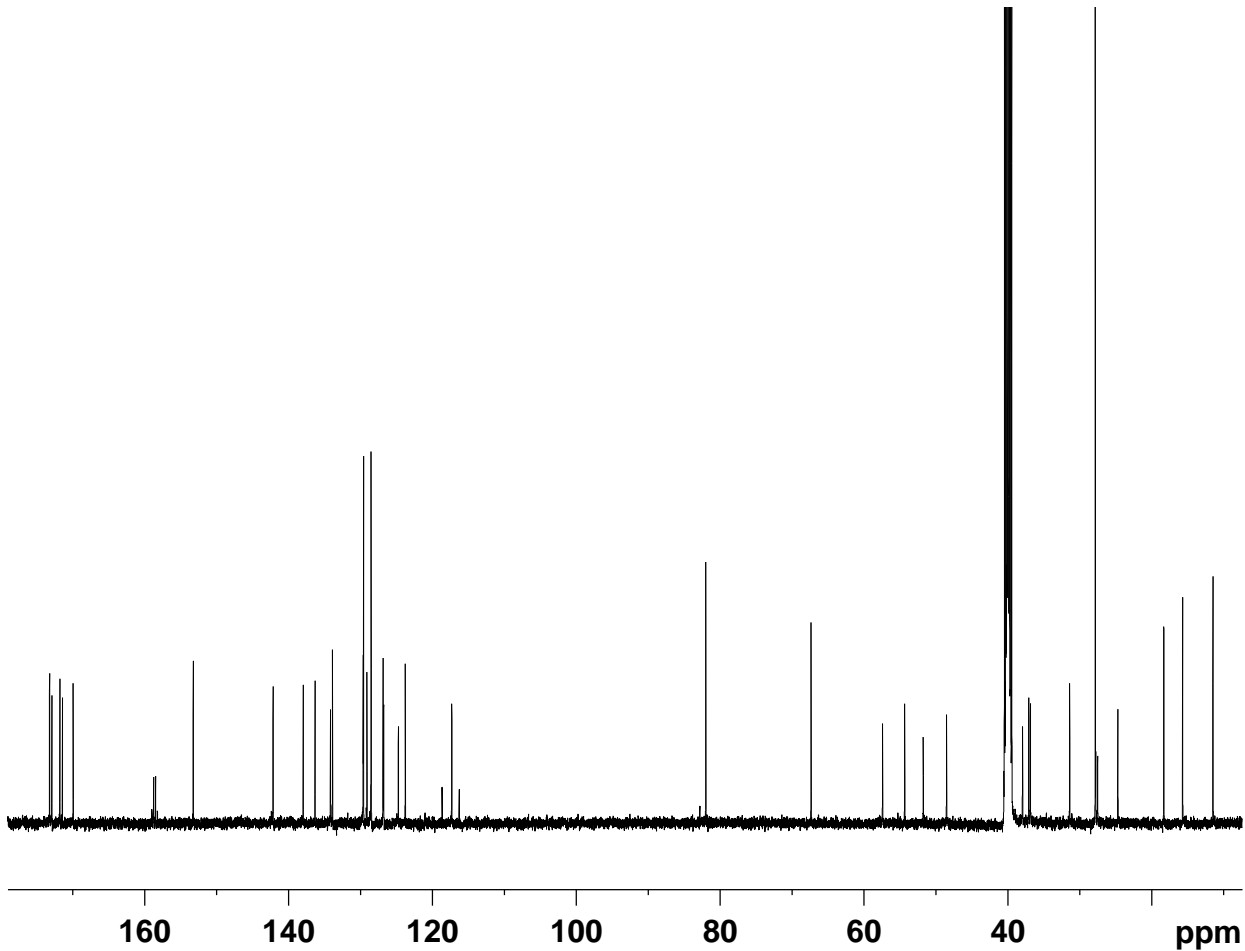
```

Current Data Parameters
NAME HIS_A6
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121130
Time 17.41
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W

F2 - Processing parameters
SI 65536
SF 500.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```



```

Current Data Parameters
NAME ICON_HISA6
EXPNO 10
PROCNO 1

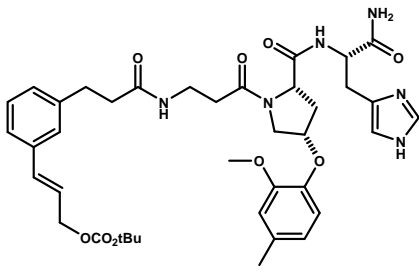
F2 - Acquisition Parameters
Date_ 20121201
Time 17.52
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7722511 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W

===== CHANNEL f2 =====
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W

F2 - Processing parameters
SI 131072
SF 125.7577892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

Acyclic-β-Ala-Pro[4-(2-methoxy-4-methylphenoxy)]-His (S27):

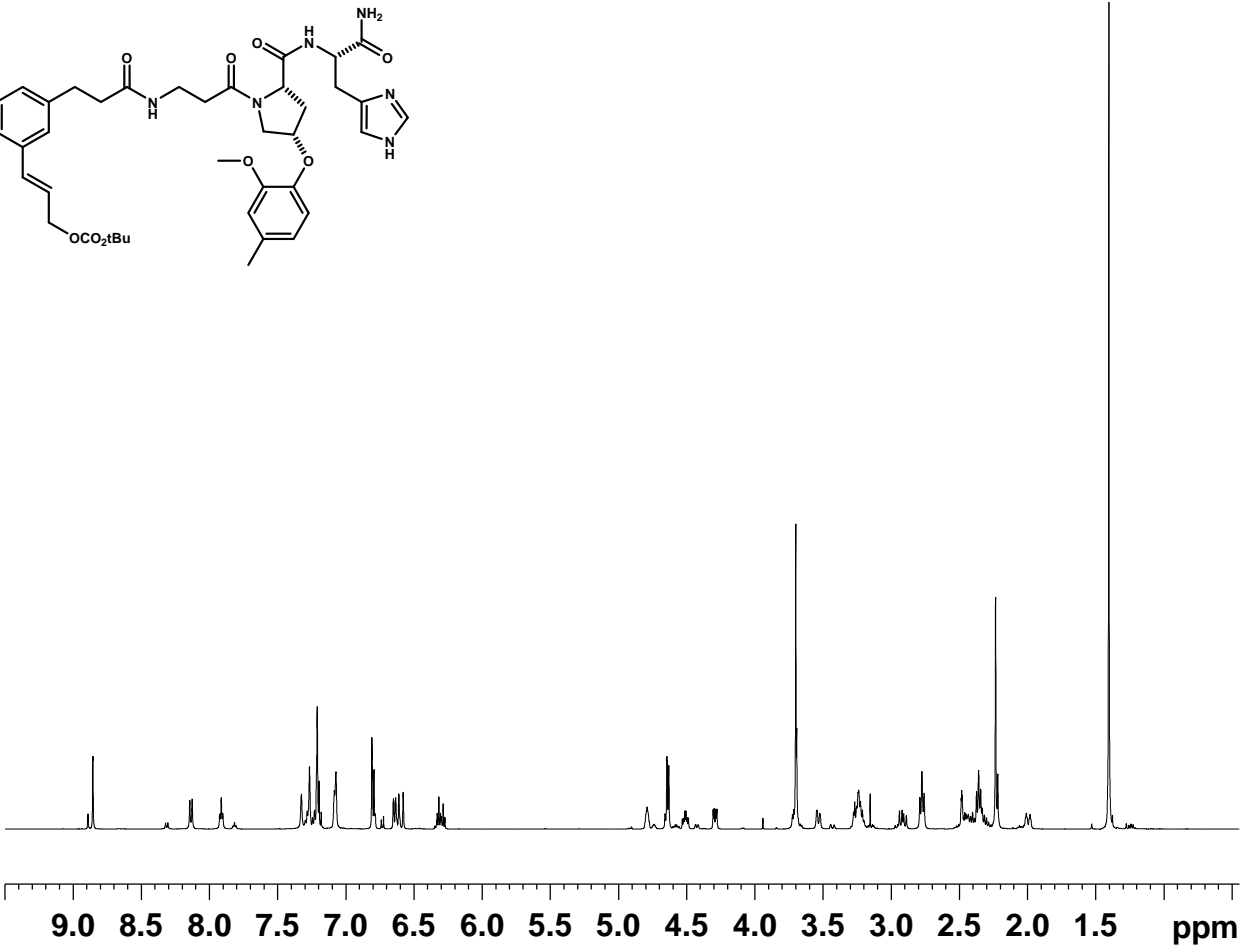


Current Data Parameters
 NAME KL-4-205
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120507
 Time 19.27
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 29.99
 DW 50.000 usec
 DE 10.00 usec
 TE 296.0 K
 D1 2.0000000 sec
 TD0 1

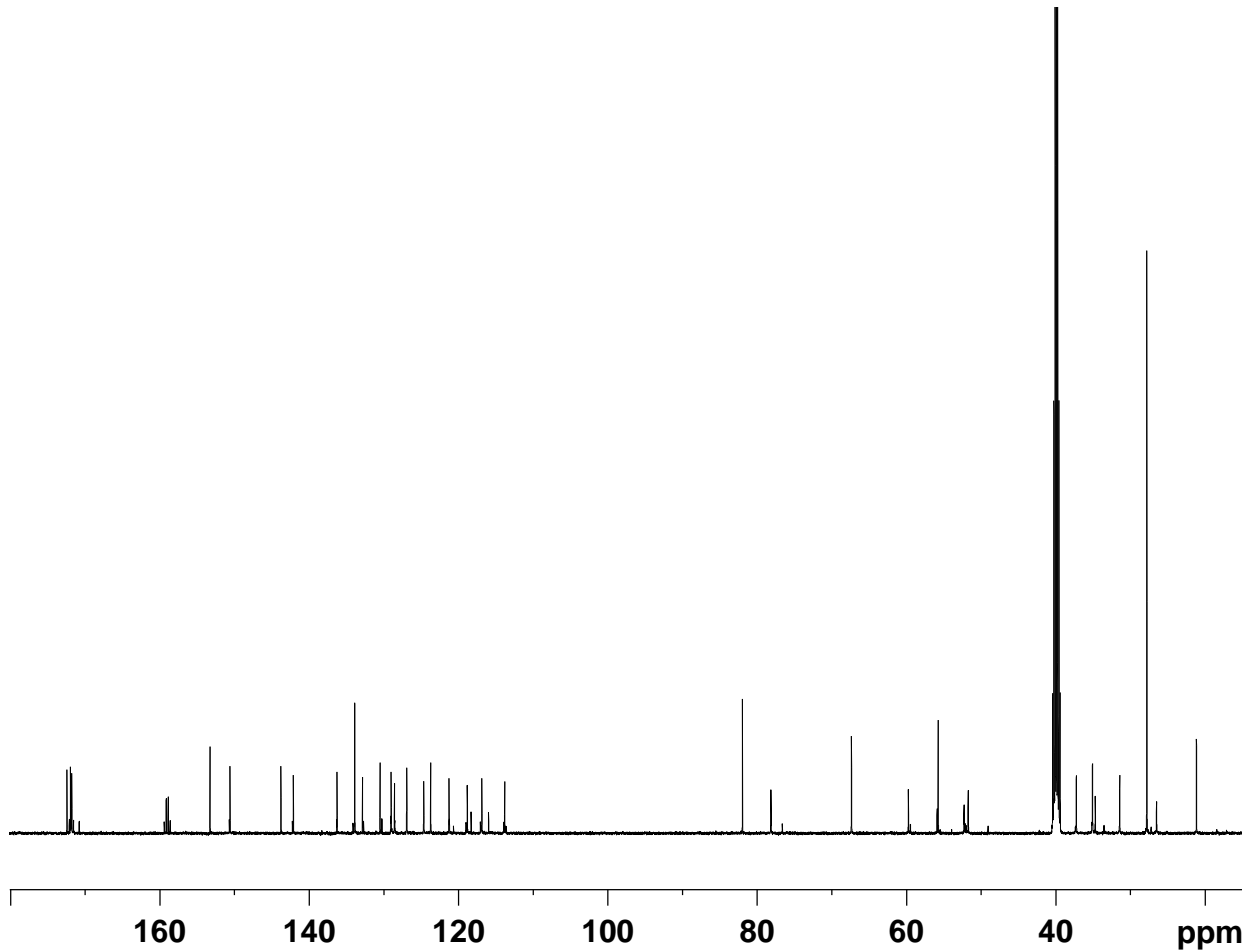
==== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PLW1 13.5000000 W
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

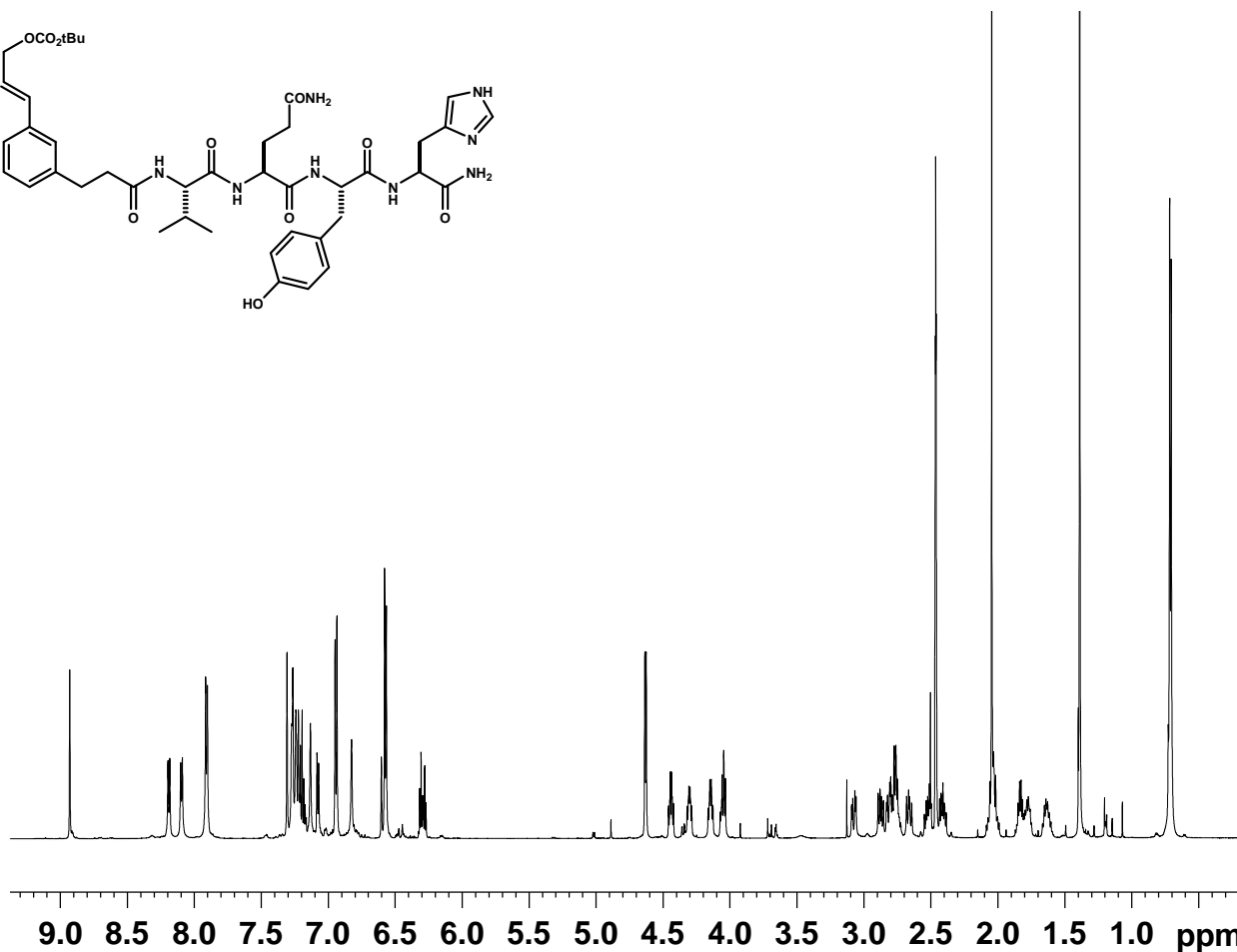
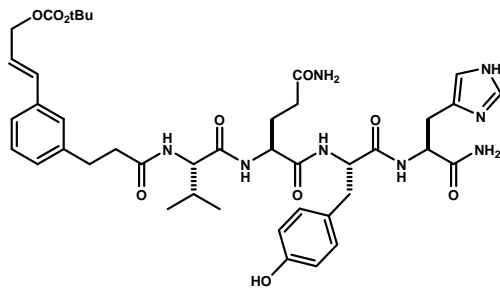


Current Data Parameters
 NAME KL-4-205
 EXPNO 2
 PROCNO 1

F2 - Processing parameters
 SI 131072
 SF 125.7577892 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Acyclic-Val-Gln-Tyr-His-NH₂ (18):

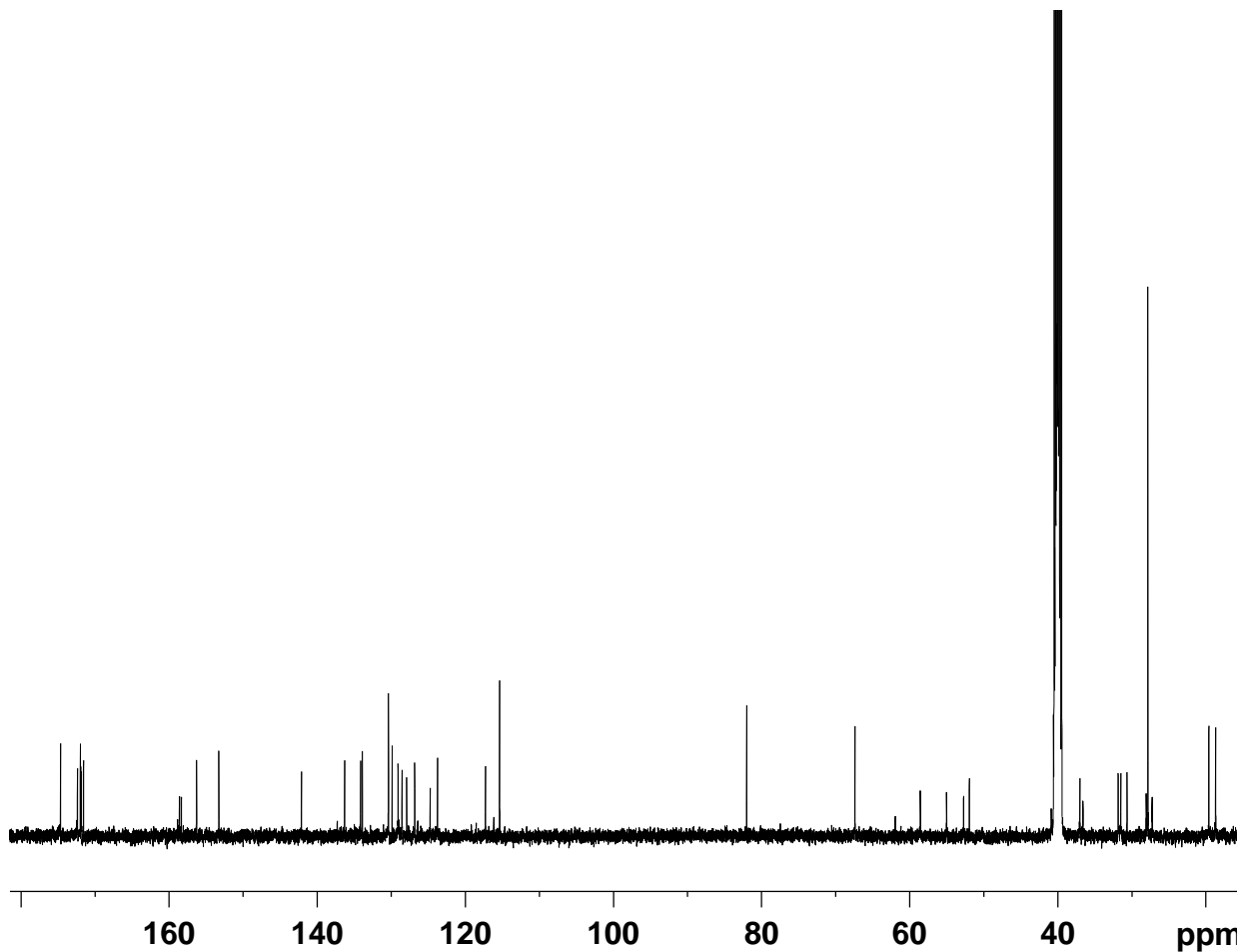


```
Current Data Parameters
NAME      KL-5-151_AV600
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20130429
Time     17.41
INSTRUM av600
PROBHD   5 mm TBI5
PULPROG zgpr
TD       65536
SOLVENT  DMSO
NS       32
DS       0
SWH      12376.237 Hz
FIDRES   0.188846 Hz
AQ       2.6476543 sec
RG       90.5
DW       40.400 usec
DE       6.50 usec
TE       293.9 K
D1       2.00000000 sec
D12      0.00002000 sec
TD0      1
```

```
===== CHANNEL f1 =====
NUC1     1H
P1       9.75 usec
PL1      -2.00 dB
PL9      52.20 dB
PL1W     39.81071854 W
PL9W     0.00015136 W
SFO1     600.1320825 MHz
```

```
F2 - Processing parameters
SI       65536
SF       600.1300273 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.40
```



```
Current Data Parameters
NAME      KL-5-151
EXPNO    3
PROCNO   1

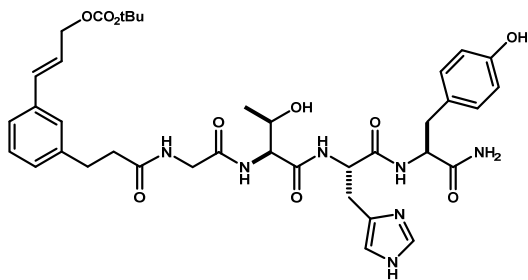
F2 - Acquisition Parameters
Date_    20130424
Time     15.43
INSTRUM av500
PROBHD   5 mm DCH 13C-1
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       126
DS       2
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0485760 sec
RG       202.91
DW       16.000 usec
DE       18.00 usec
TE       298.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
```

```
===== CHANNEL f1 =====
SFO1     125.7722511 MHz
NUC1     13C
P1       9.63 usec
PLW1     23.00000000 W
```

```
===== CHANNEL f2 =====
SFO2     500.1330008 MHz
NUC2     1H
CPDPRG[2] waltz16
PCPD2    80.00 usec
PLW2     13.50000000 W
PLW12    0.21094000 W
PLW13    0.13500001 W
```

```
F2 - Processing parameters
SI       131072
SF       125.7577892 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

Acyclic-Gly-Thr-His-Tyr-NH₂ (S29):



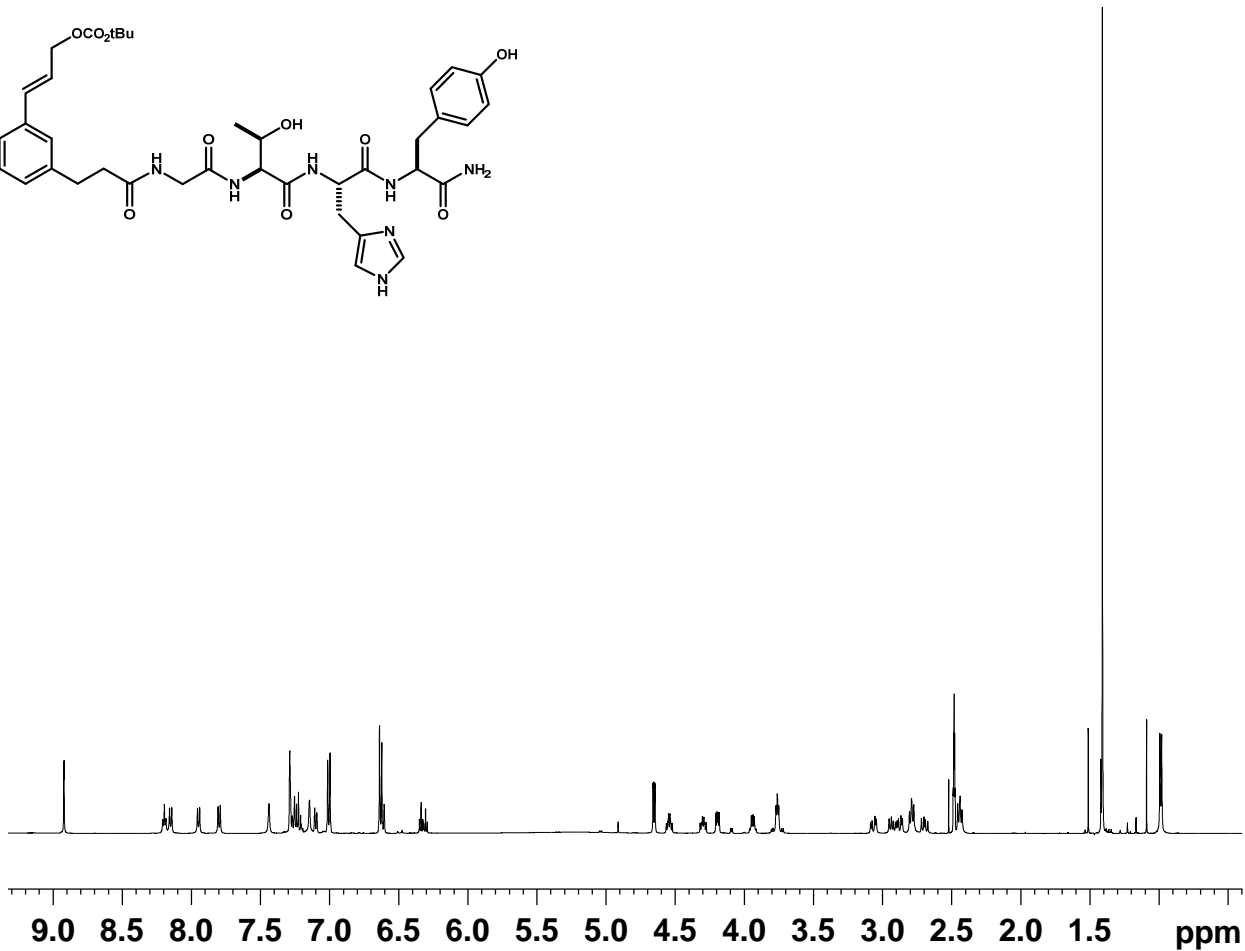
```

Current Data Parameters
NAME HIS_A2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121130
Time 17.28
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W

F2 - Processing parameters
SI 65536
SF 500.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```



```

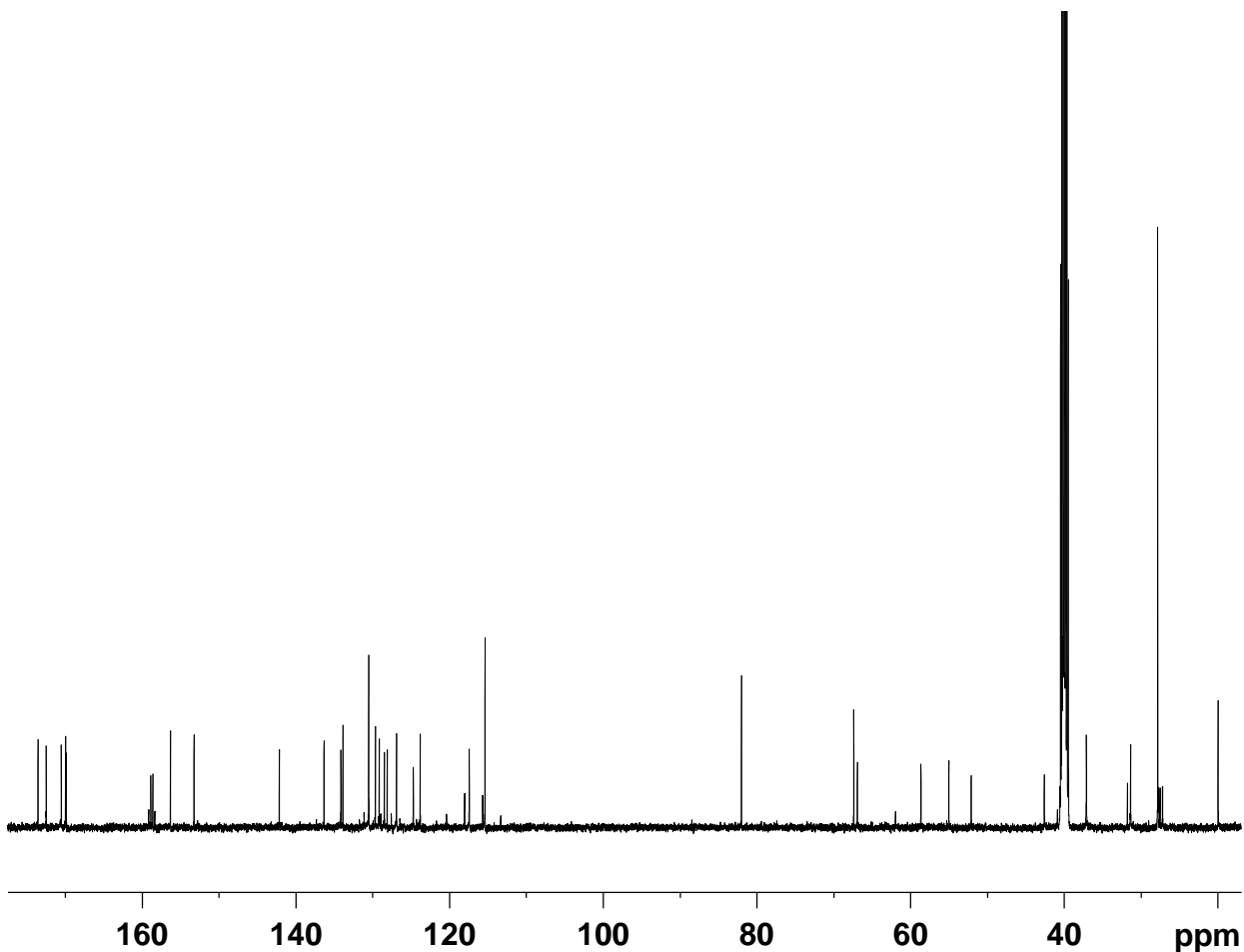
Current Data Parameters
NAME ICON_HISA2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121201
Time 17.27
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

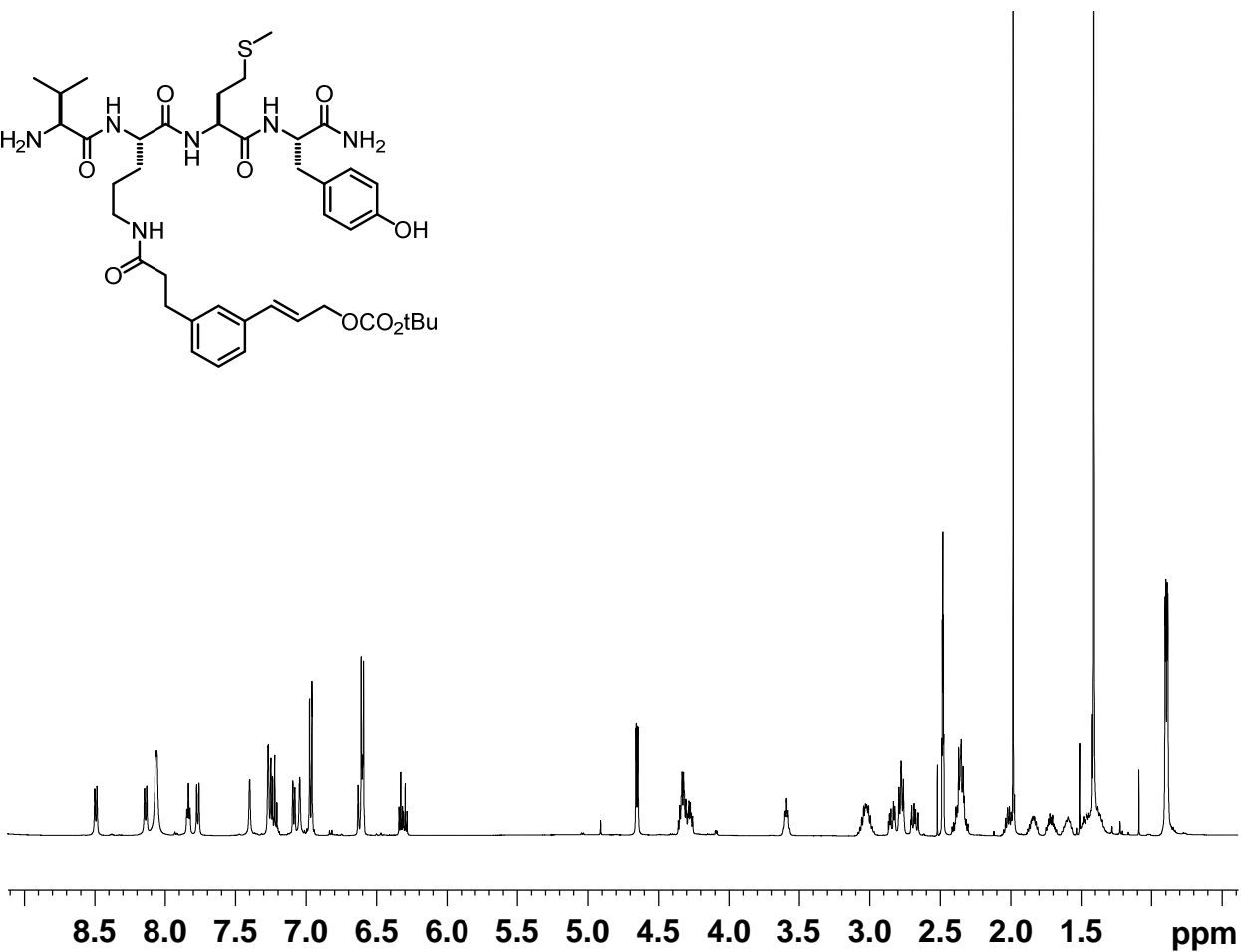
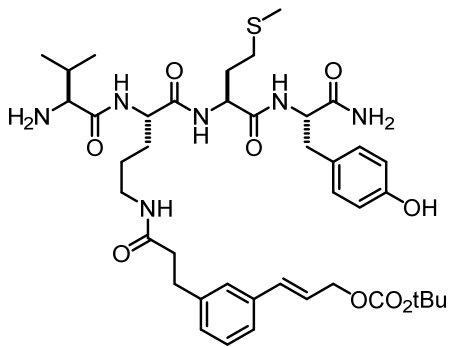
===== CHANNEL f1 =====
SFO1 125.7722511 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W

===== CHANNEL f2 =====
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W

F2 - Processing parameters
SI 131072
SF 125.7577892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```



Acyclic-Val-Orn-Met-Tyr (S30):



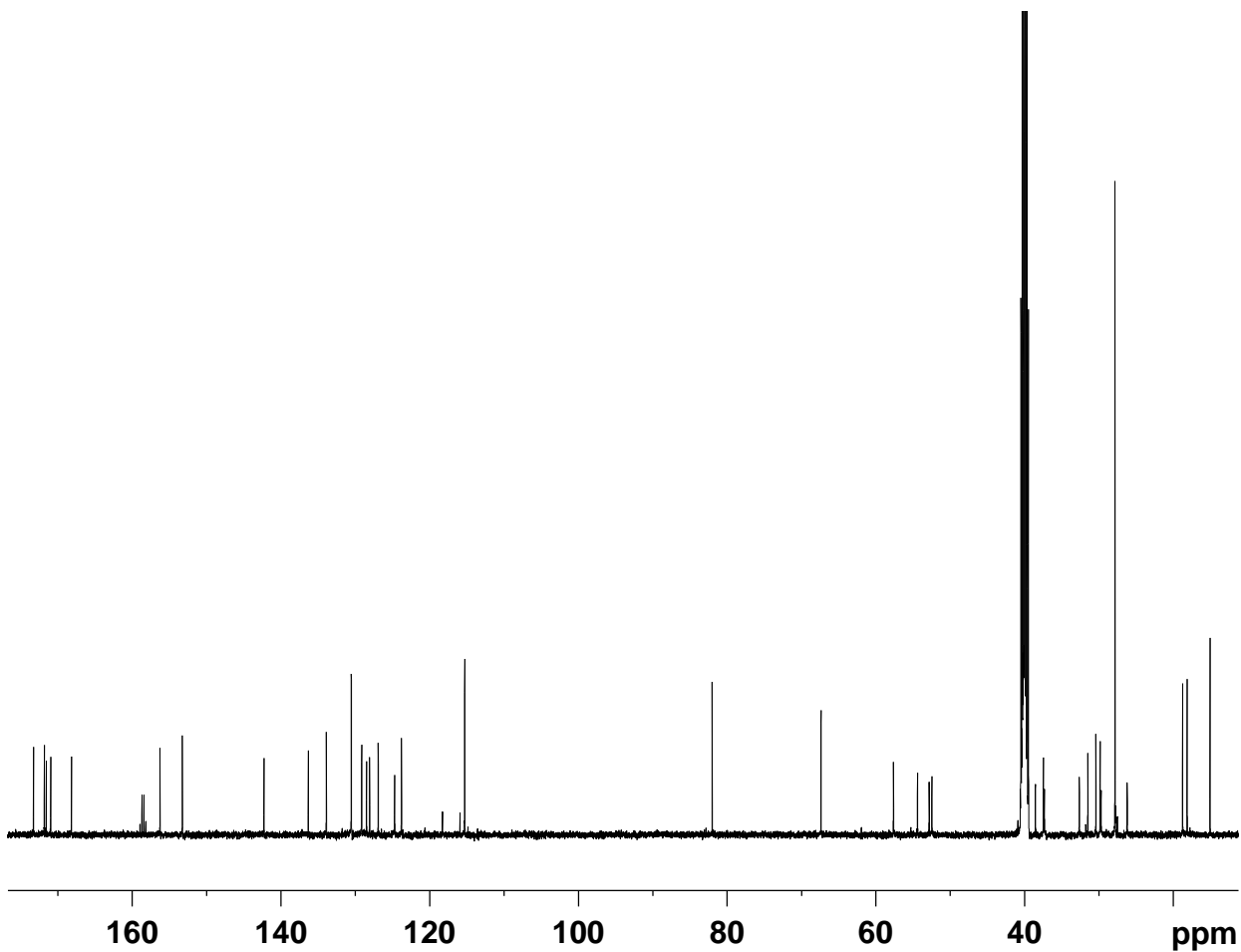
```

Current Data Parameters
NAME      KL-5-153_deprot
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130409
Time     12.12
INSTRUM av500
PROBHD   5 mm DCH 13C-1
PULPROG zg30
TD       65536
SOLVENT  DMSO
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       11
DW       50.000 usec
DE       10.00 usec
TE       298.0 K
D1       2.0000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    500.1330008 MHz
NUC1     1H
P1       10.00 usec
PLW1    13.5000000 W

F2 - Processing parameters
SI       65536
SF       500.1300146 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



```

Current Data Parameters
NAME      KL-5-153_deprot
EXPNO    2
PROCNO   1

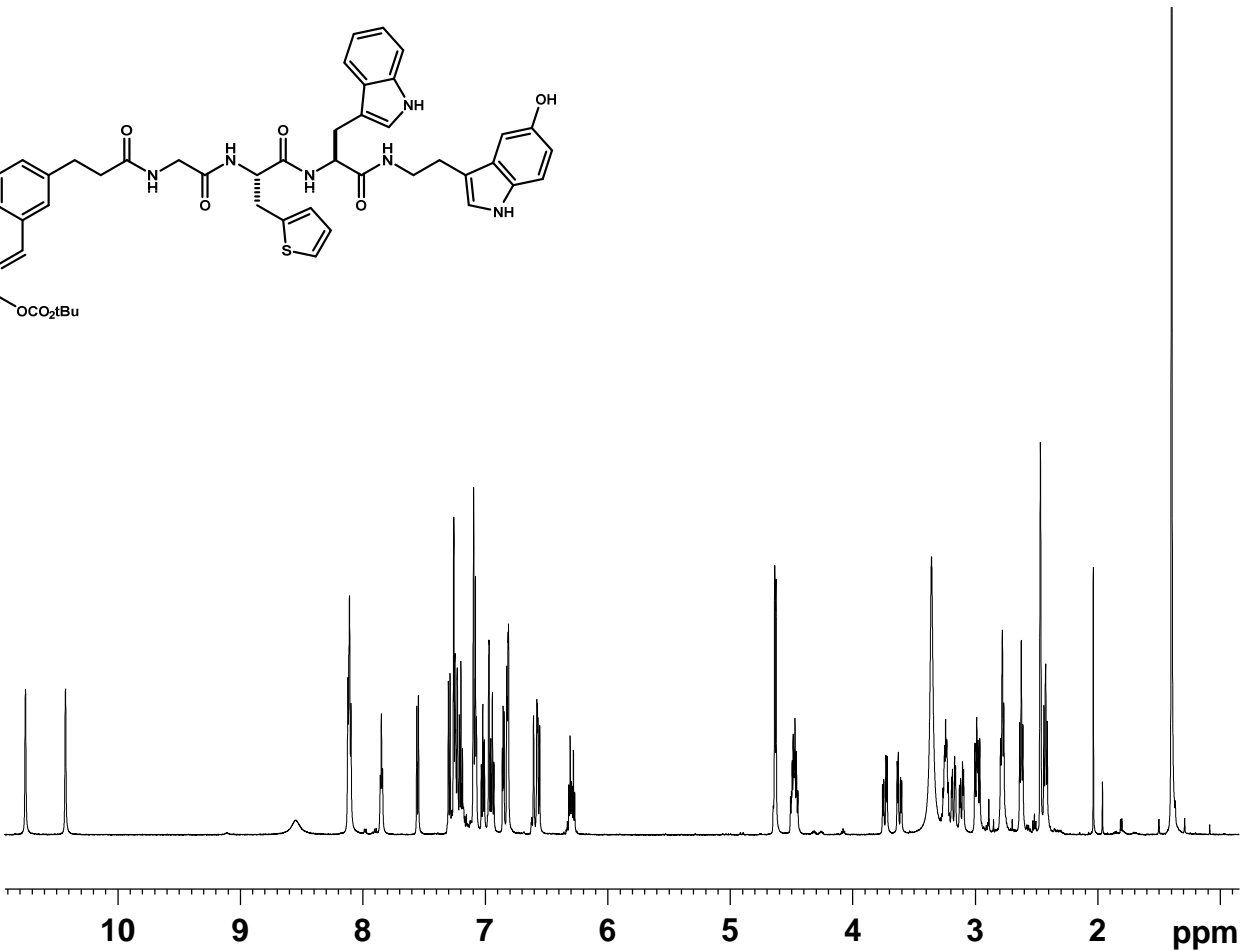
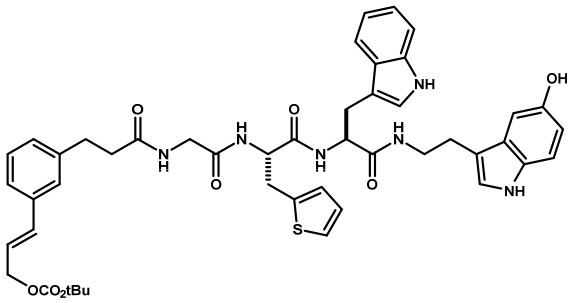
F2 - Acquisition Parameters
Date_    20130409
Time     12.15
INSTRUM av500
PROBHD   5 mm DCH 13C-1
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       85
DS       2
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0485760 sec
RG       202.91
DW       16.000 usec
DE       18.00 usec
TE       298.0 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    125.7722511 MHz
NUC1     13C
P1       9.63 usec
PLW1    23.0000000 W

===== CHANNEL f2 =====
SFO2    500.1330008 MHz
NUC2     1H
CPDPRG[2] waltz16
PCPD2   80.00 usec
PLW2    13.5000000 W
PLW12   0.21094000 W
PLW13   0.13500001 W

F2 - Processing parameters
SI       131072
SF       125.7577892 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

Acyclic-Gly-Thi-Trp-5HT (S31):



```

Current Data Parameters
NAME          KL-4-46
EXPNO        2
PROCNO       1

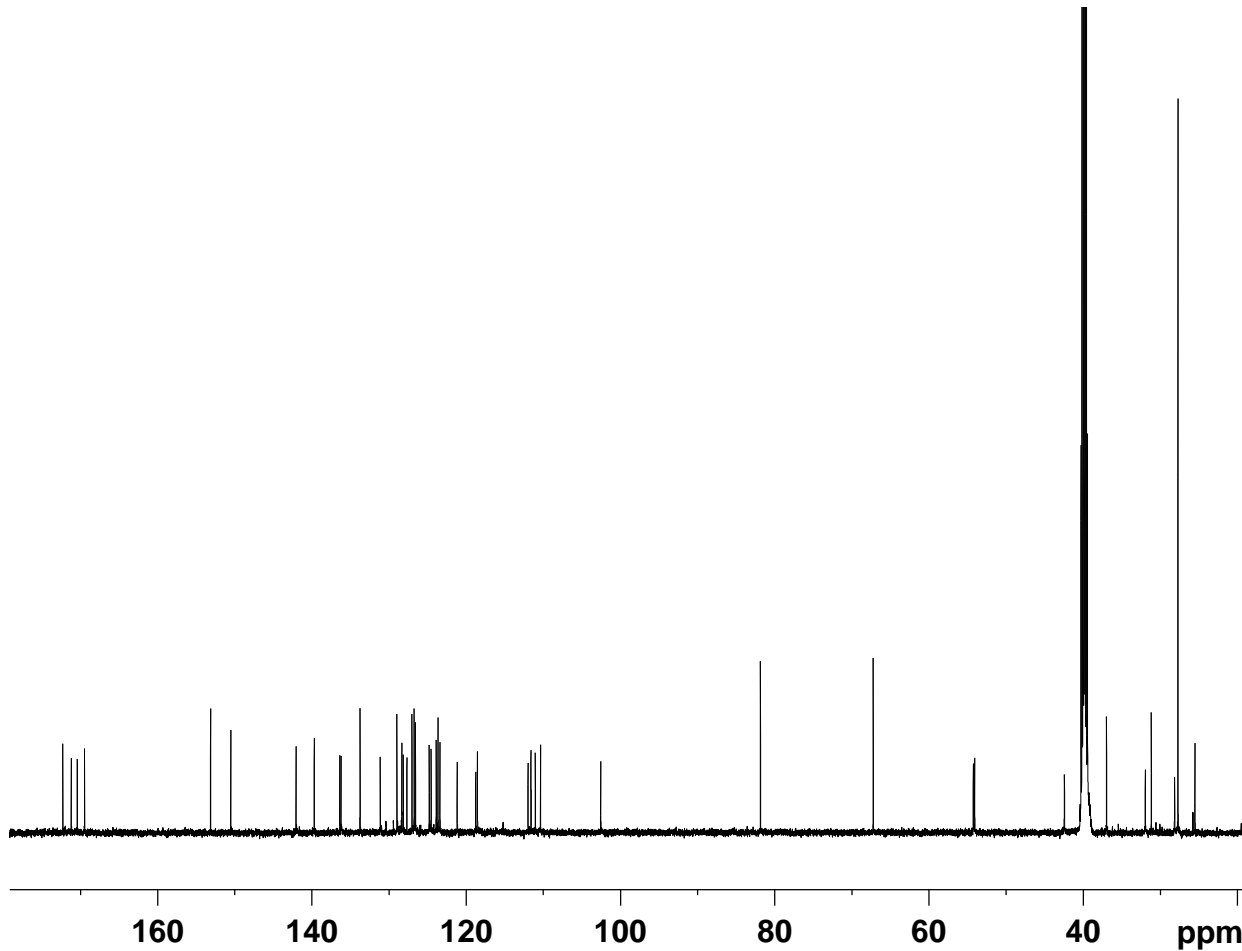
F2 - Acquisition Parameters
Date_        2011012
Time         15.55
INSTRUM     av600
PROBHD      5 mm BB5
PULPROG     zg30
TD          65536
SOLVENT     DMSO
NS          4
DS          0
SWH         12376.237 Hz
FIDRES     0.188846 Hz
AQ         2.6476543 sec
RG          90.5
DW         40.400 usec
DE          6.50 usec
TE         300.5 K
D1         2.0000000 sec
TD0        1
    
```

```

===== CHANNEL f1 =====
NUC1        1H
P1          14.00 usec
PL1         -1.00 dB
PL1W       31.62277603 W
SFO1       600.1336008 MHz
    
```

```

F2 - Processing parameters
SI          65536
SF         600.1300273 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
    
```



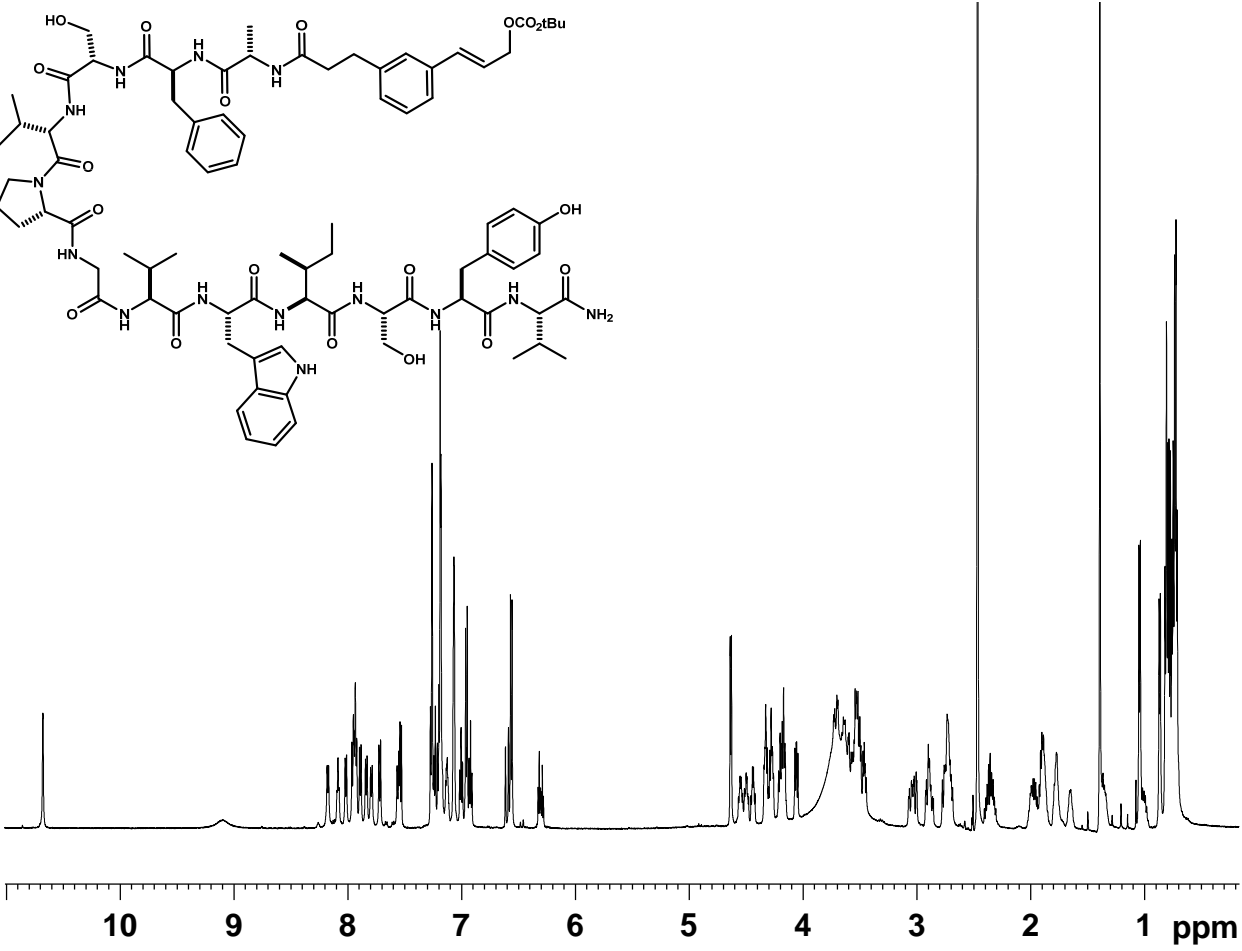
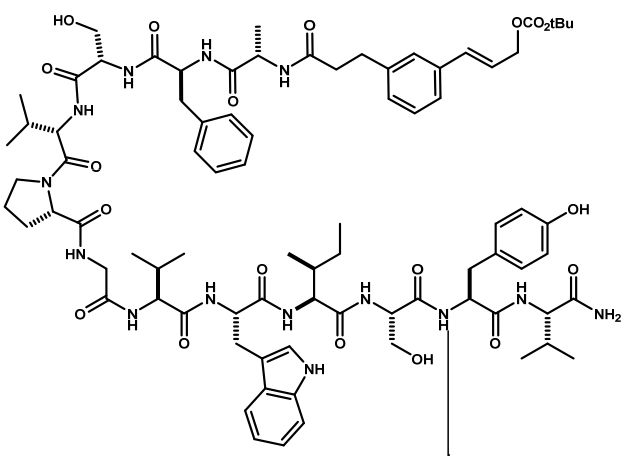
```

Current Data Parameters
NAME          KL-4-46
EXPNO        3
PROCNO       1
    
```

```

F2 - Processing parameters
SI          65536
SF         150.9028319 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

Acyclic-Ala-Phe-Ser-Val-Pro-Gly-Val-Trp-Ile-Ser-Tyr-Val (S32):

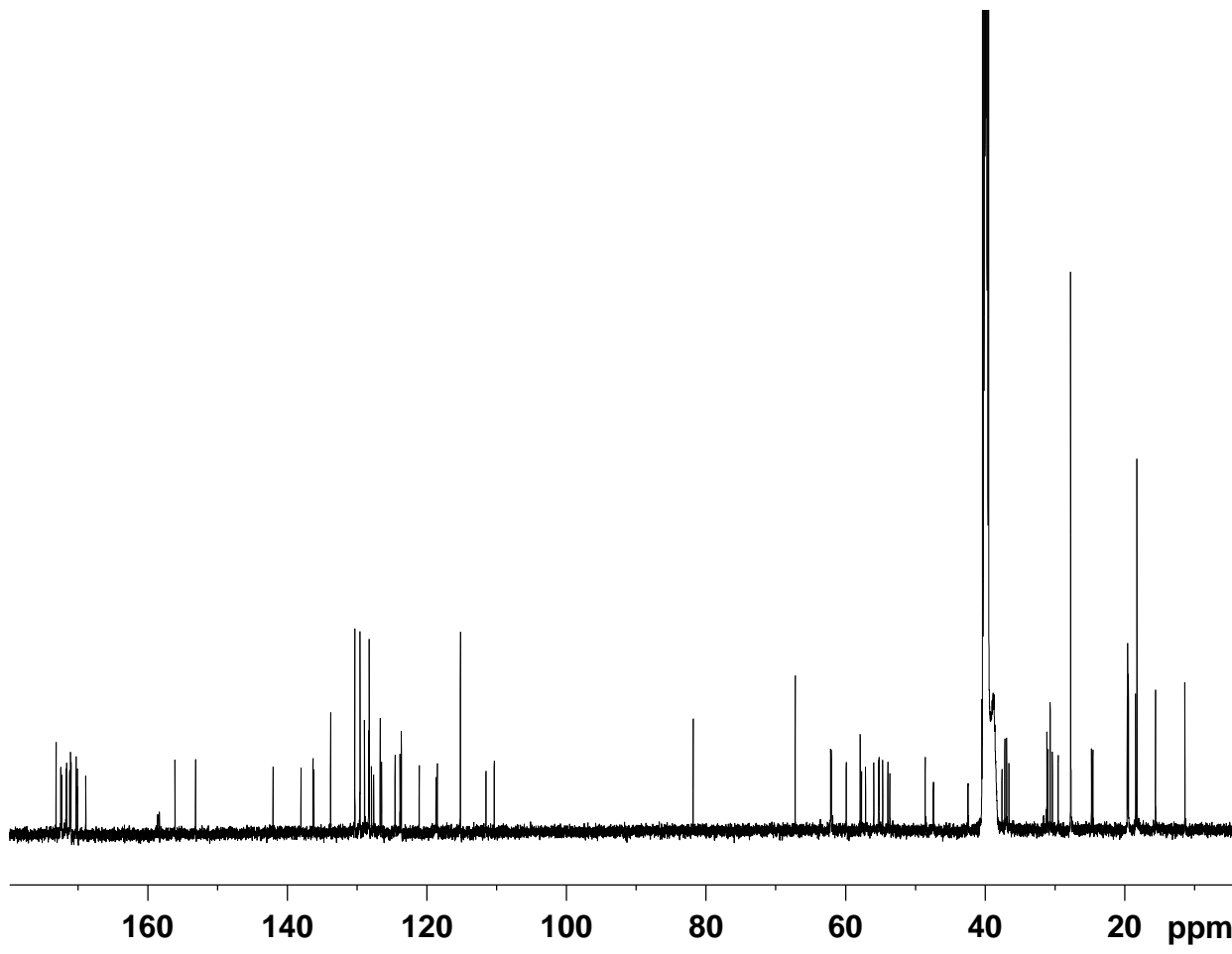


Current Data Parameters
 NAME KL-4-7_prep
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110923
 Time 14.35
 INSTRUM av600
 PROBHD 5 mm TBI5
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 12376.237 Hz
 FIDRES 0.188846 Hz
 AQ 2.6476543 sec
 RG 114
 DW 40.400 usec
 DE 6.50 usec
 TE 294.3 K
 DL 2.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.10 usec
 PL1 -2.00 dB
 PLLW 39.81071854 W
 SFO1 600.1336008 MHz

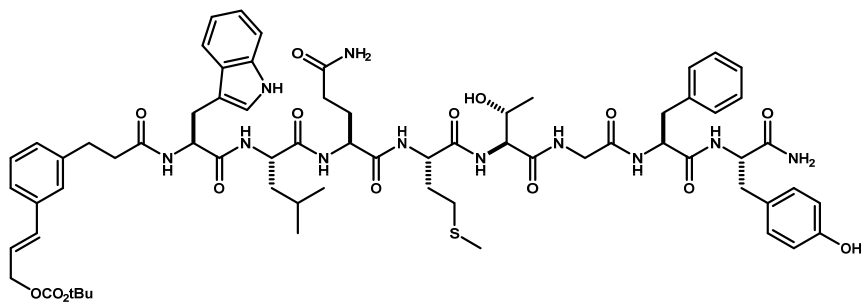
F2 - Processing parameters
 SI 65536
 SF 600.1300273 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-4-7_prep
 EXPNO 3
 PROCNO 1

F2 - Processing parameters
 SI 65536
 SF 150.9028319 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

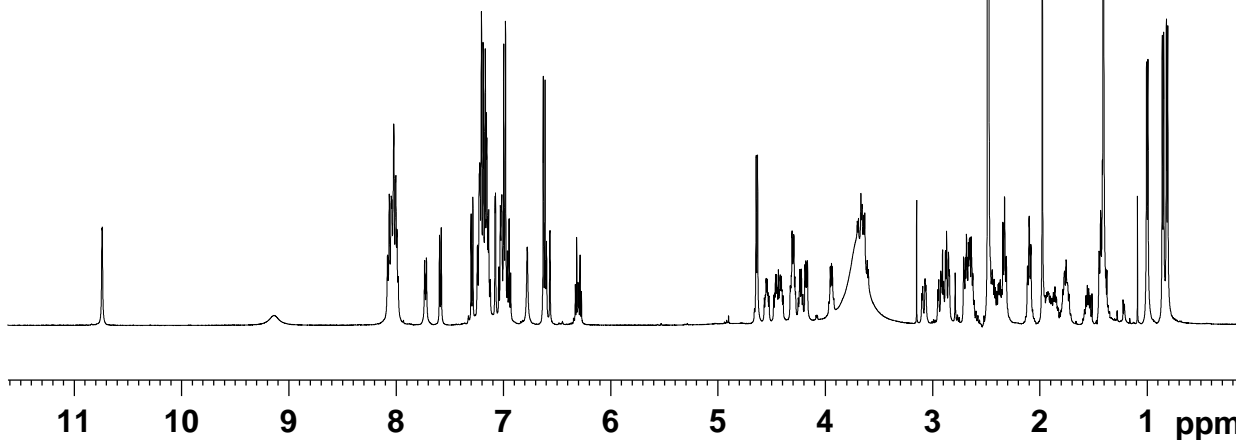
Acyclic-Trp-Leu-Gln-Met-Thr-Gly-Phe-Tyr (S33):



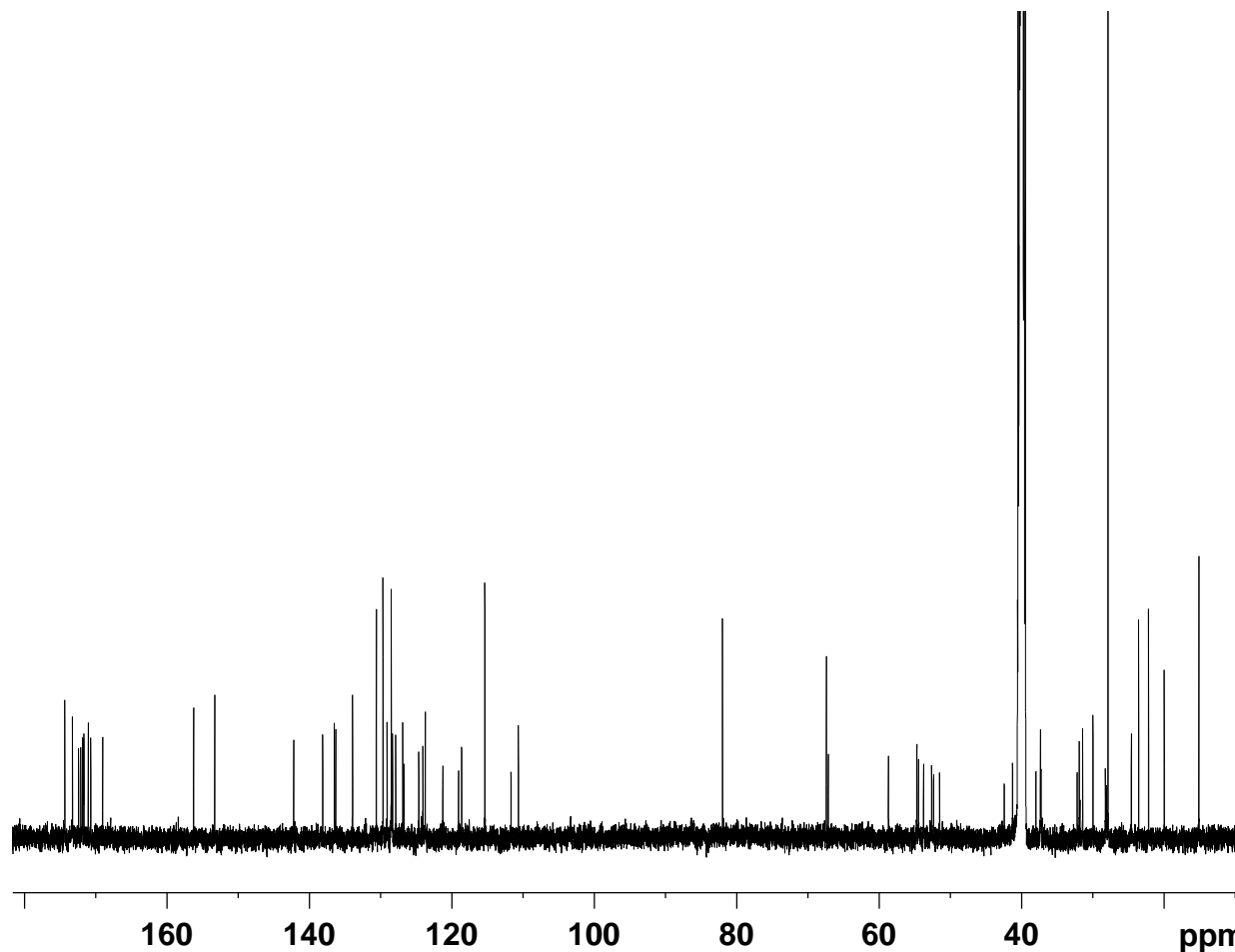
Current Data Parameters
 NAME KL-4-15d_F21
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20120730
 Time 12.13
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 202.91
 DW 50.000 usec
 DE 10.00 usec
 TE 296.0 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PLW1 13.5000000 W
 SFO1 500.1330008 MHz

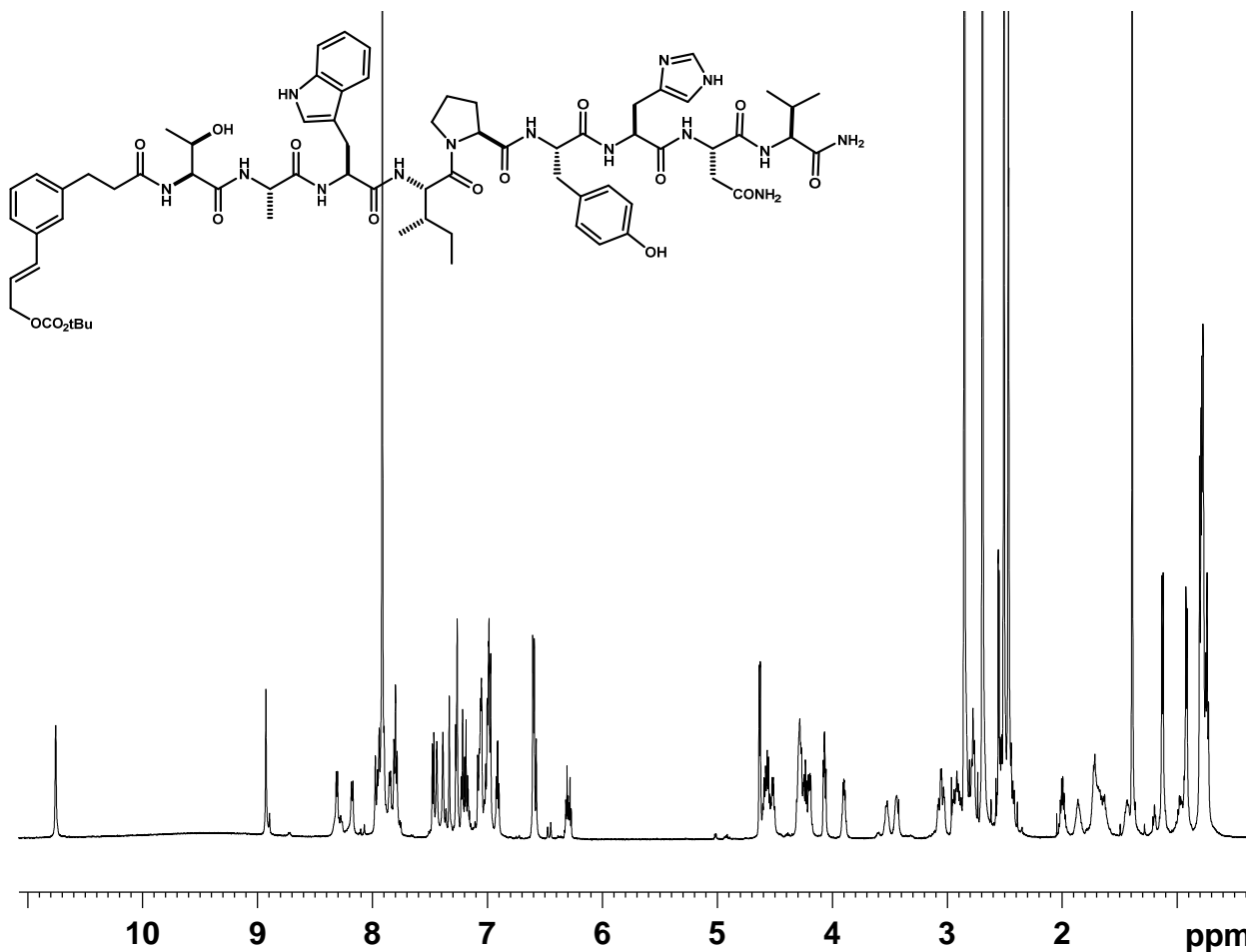
F2 - Processing parameters
 SI 65536
 SF 500.1300146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-4-15d_F21
 EXPNO 2
 PROCNO 1
 F2 - Processing parameters
 SI 131072
 SF 125.7577892 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



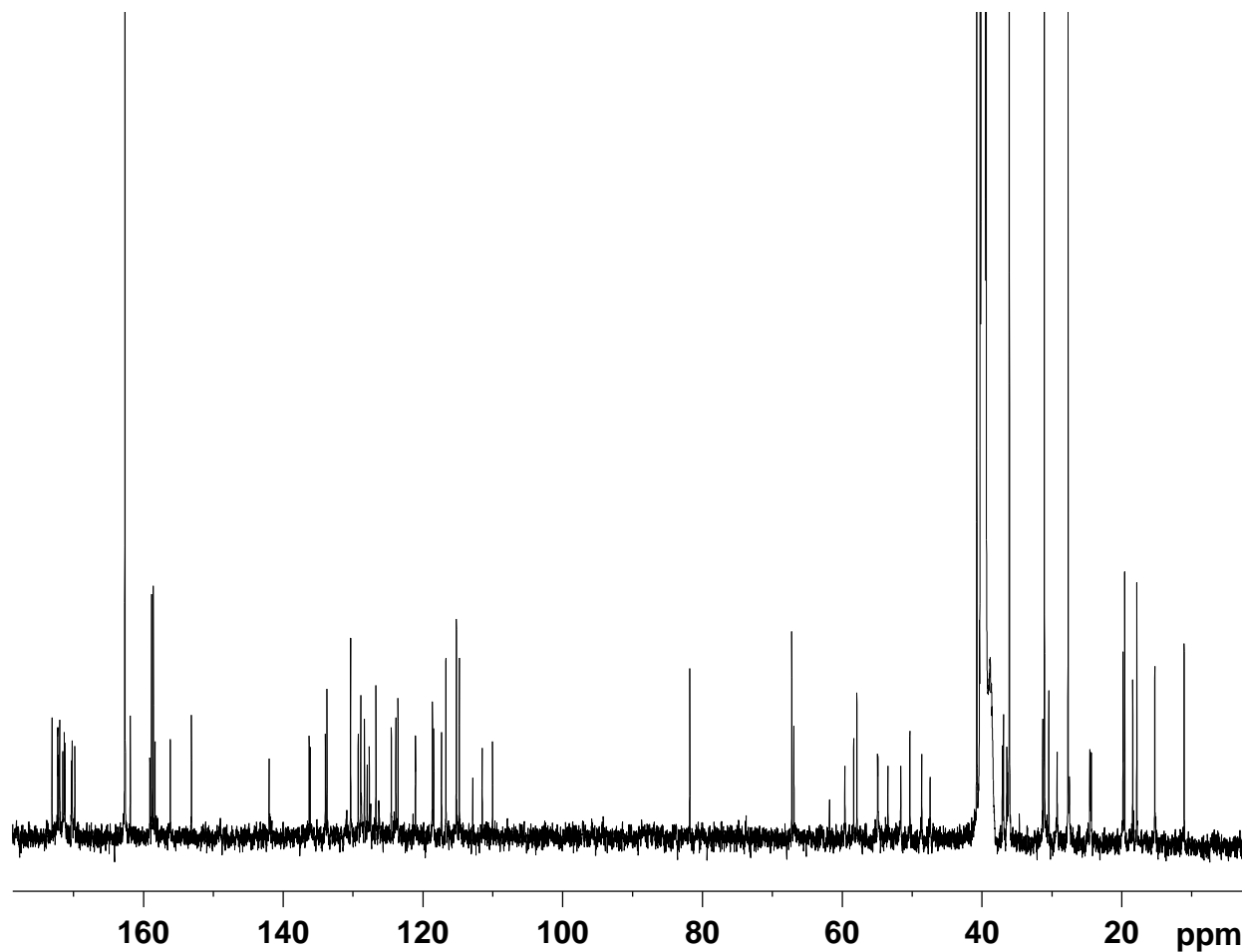
Acyclic-Thr-Ala-Trp-Ile-Pro-Tyr-His-Asn-Val (S34):



Current Data Parameters
 NAME KL-III-284
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110829
 Time 17.20
 INSTRUM av600
 PROBHD 5 mm BB5
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 12376.237 Hz
 FIDRES 0.188846 Hz
 AQ 2.6476543 sec
 RG 90.5
 DW 40.400 usec
 DE 6.50 usec
 TE 294.5 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 -1.00 dB
 PL1W 31.62277603 W
 SFO1 600.1336008 MHz

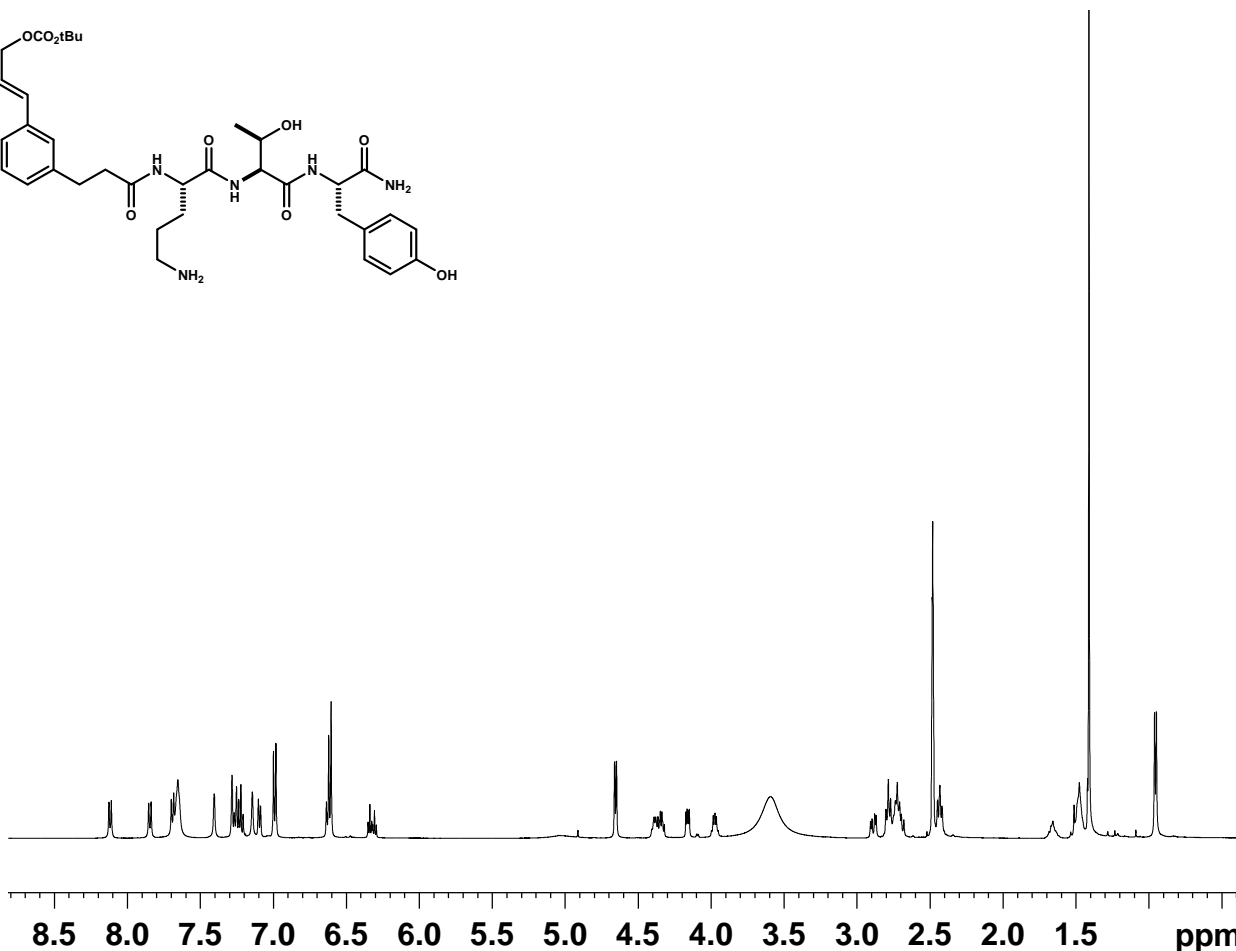
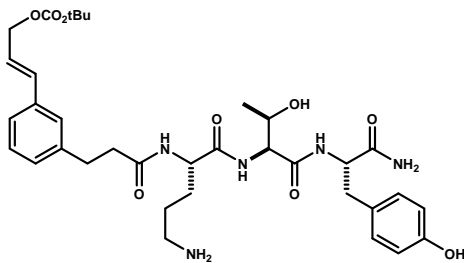
F2 - Processing parameters
 SI 65536
 SF 600.1300273 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME KL-III-284
 EXPNO 2
 PROCNO 1

F2 - Processing parameters
 SI 65536
 SF 150.9028319 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Acyclic-Orn-Thr-Tyr (S35):

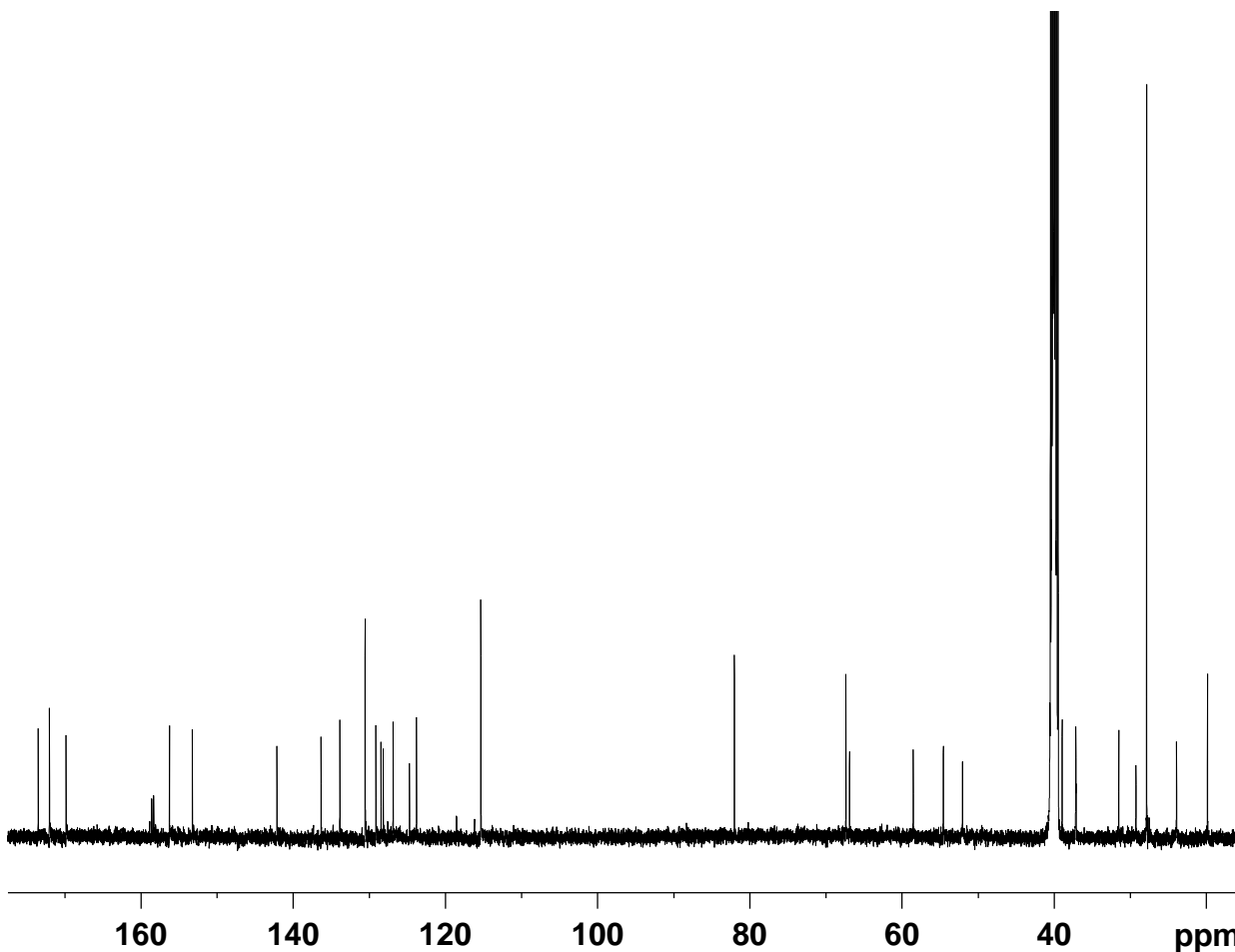


```
Current Data Parameters
NAME TR4-128
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130322
Time 20.59
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 11
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W
```

```
F2 - Processing parameters
SI 65536
SF 500.1300146 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
```



```
Current Data Parameters
NAME TR4-128
EXPNO 2
PROCNO 1

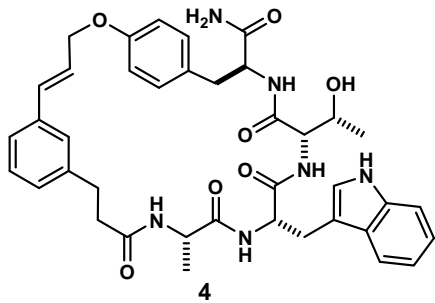
F2 - Acquisition Parameters
Date_ 20130322
Time 21.02
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 15.53
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
SFO1 125.7722511 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
```

```
===== CHANNEL f2 =====
SFO2 500.1330008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
```

```
F2 - Processing parameters
SI 131072
SF 125.7577892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
```

Cyclic-Ala-Trp-Thr-Tyr (4):



```

Current Data Parameters
NAME      KL-4-55_CHECK
EXPNO     1
PROCNO    1

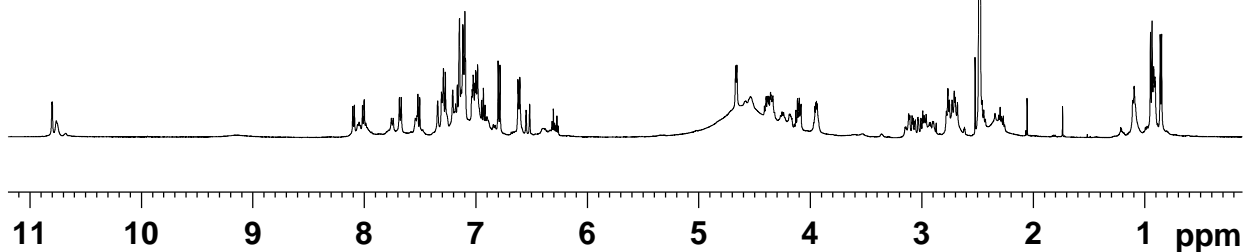
F2 - Acquisition Parameters
Date_     2011019
Time      19.56
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zg30
TD         65536
SOLVENT    DMSO
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2767999 sec
RG         22.82
DW         50.000 usec
DE         10.00 usec
TE         301.0 K
D1         2.0000000 sec
TD0        1
    
```

```

===== CHANNEL f1 =====
NUC1       1H
P1         10.00 usec
PLW1       13.5000000 W
SFO1       500.1330008 MHz
    
```

```

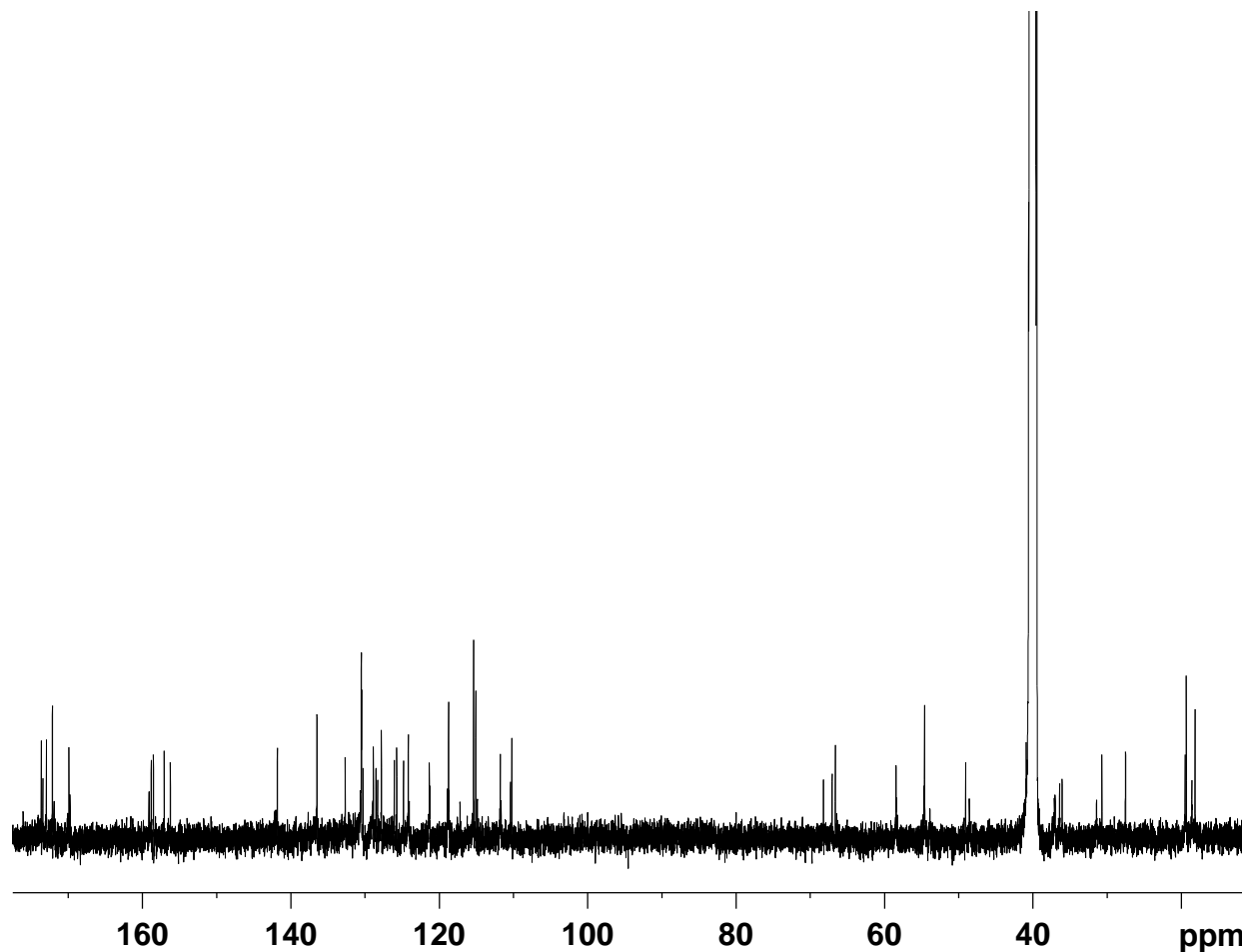
F2 - Processing parameters
SI         65536
SF         500.1300146 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



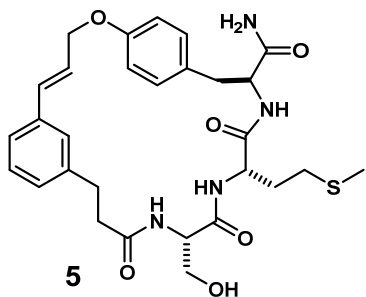
```

Current Data Parameters
NAME      KL-4-55_CHECK
EXPNO     2
PROCNO    1

F2 - Processing parameters
SI         131072
SF         125.7577892 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
    
```



Cyclic-Ser-Met-Tyr (5):



```

Current Data Parameters
NAME          KL-4-16
EXPNO         1
PROCNO        1

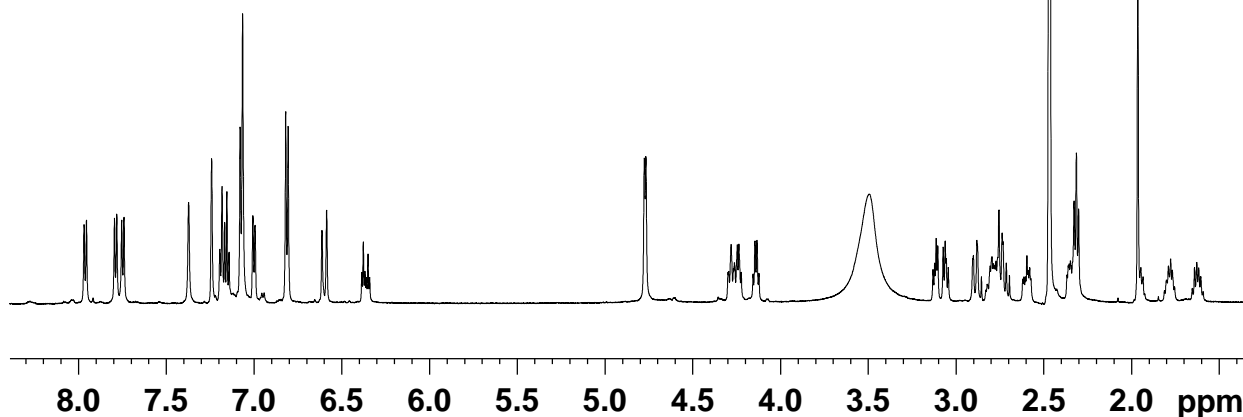
F2 - Acquisition Parameters
Date_         20110926
Time          16.58
INSTRUM       av600
PROBHD        5 mm TBI5
PULPROG       zg30
TD             65536
SOLVENT       DMSO
NS             8
DS             0
SWH            12376.237 Hz
FIDRES         0.188846 Hz
AQ             2.6476543 sec
RG             181
DW             40.400 usec
DE             6.50 usec
TE             294.0 K
D1             2.0000000 sec
TD0            1
    
```

```

===== CHANNEL f1 =====
NUC1           1H
P1              9.10 usec
PL1             -2.00 dB
PL1W            39.81071854 W
SF01            600.1336008 MHz
    
```

```

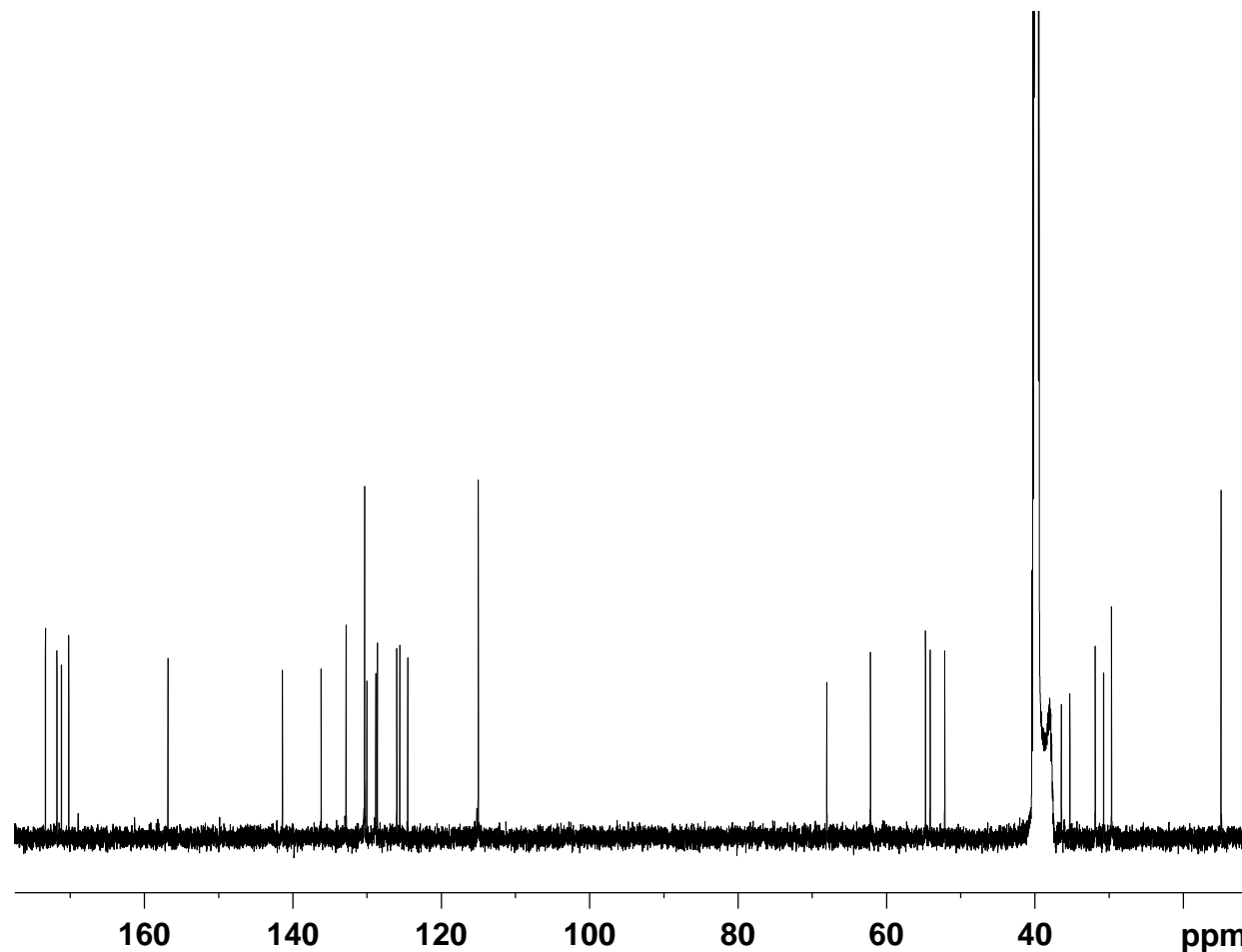
F2 - Processing parameters
SI              65536
SF              600.1300273 MHz
WDW             EM
SSB             0
LB              0.30 Hz
GB              0
PC              1.00
    
```



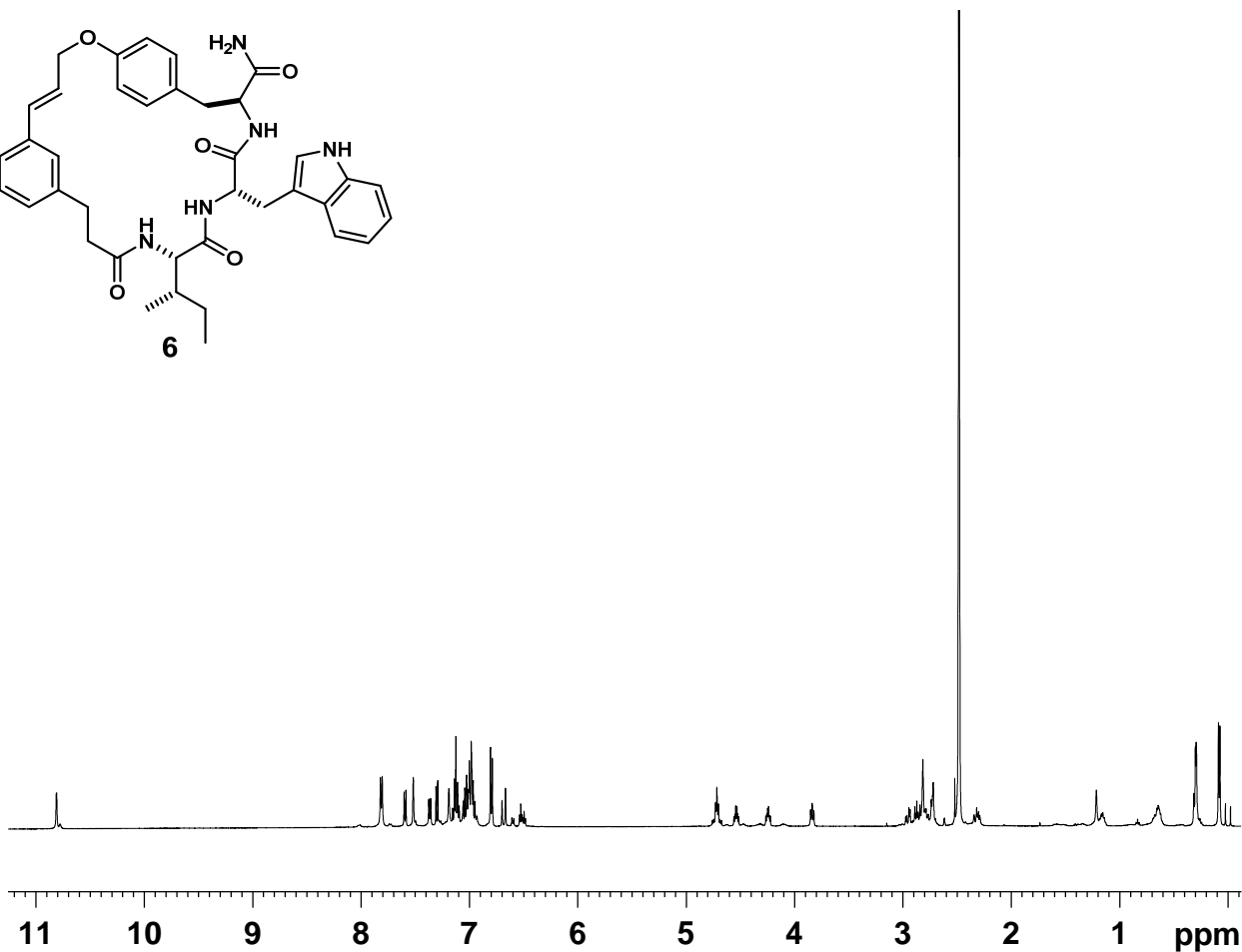
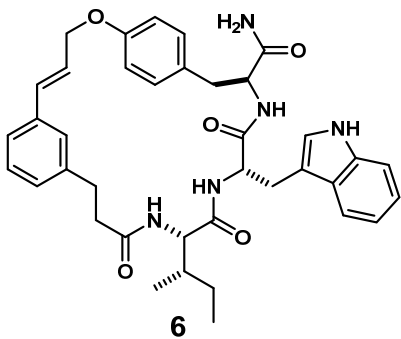
```

Current Data Parameters
NAME          KL-4-16
EXPNO         3
PROCNO        1

F2 - Processing parameters
SI              65536
SF              150.9028319 MHz
WDW             EM
SSB             0
LB              1.00 Hz
GB              0
PC              1.40
    
```



Cyclic-Ile-Trp-Tyr (6):



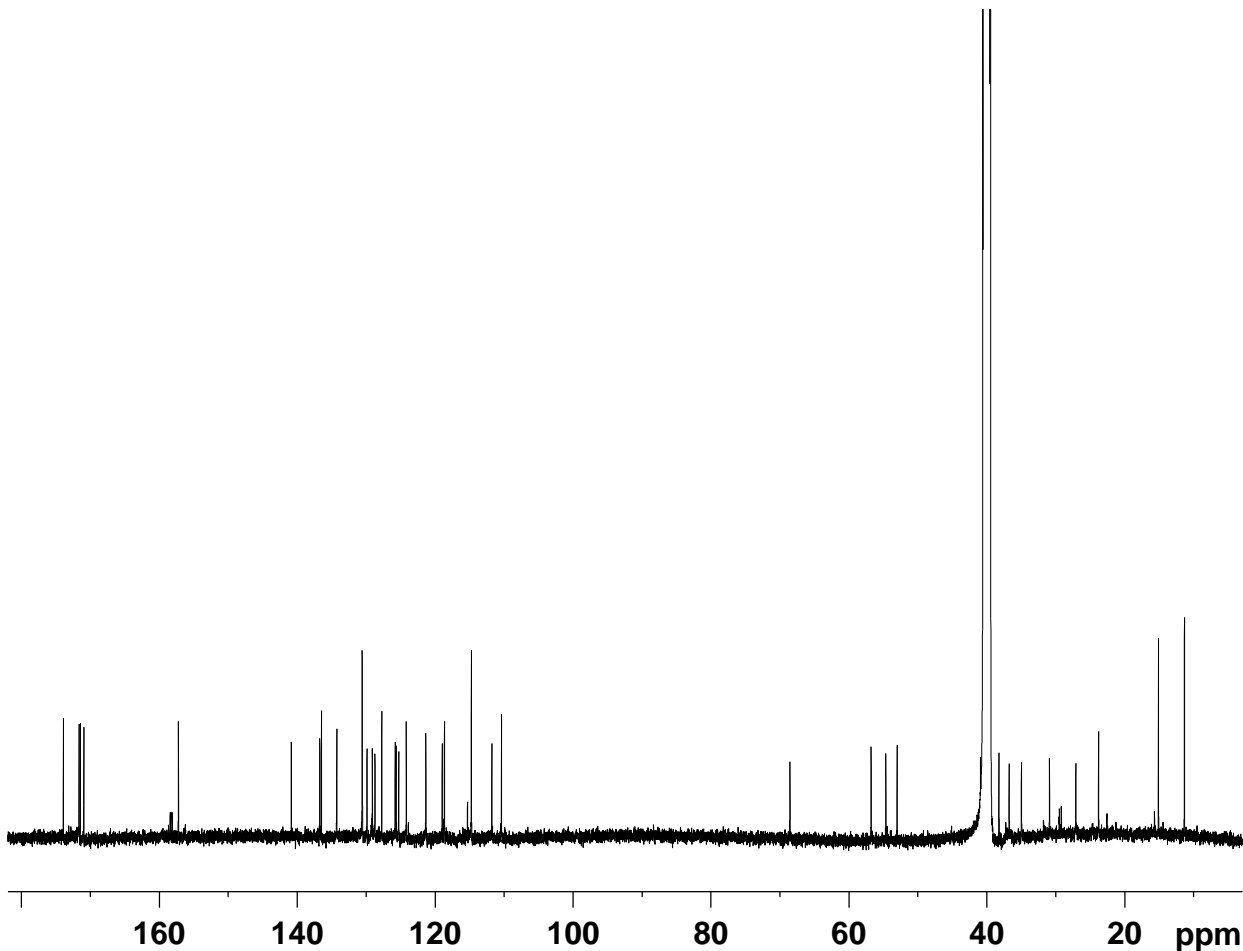
```

Current Data Parameters
NAME          IWY-Cy
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20130509
Time          11.10
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpr
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            11
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.00000000 sec
D12           0.00002000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          500.1317204 MHz
NUC1          1H
P1            10.00 usec
PLW1          13.50000000 W
PLW9          0.00005400 W

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



```

Current Data Parameters
NAME          IWY-Cy
EXPNO         6
PROCNO        1

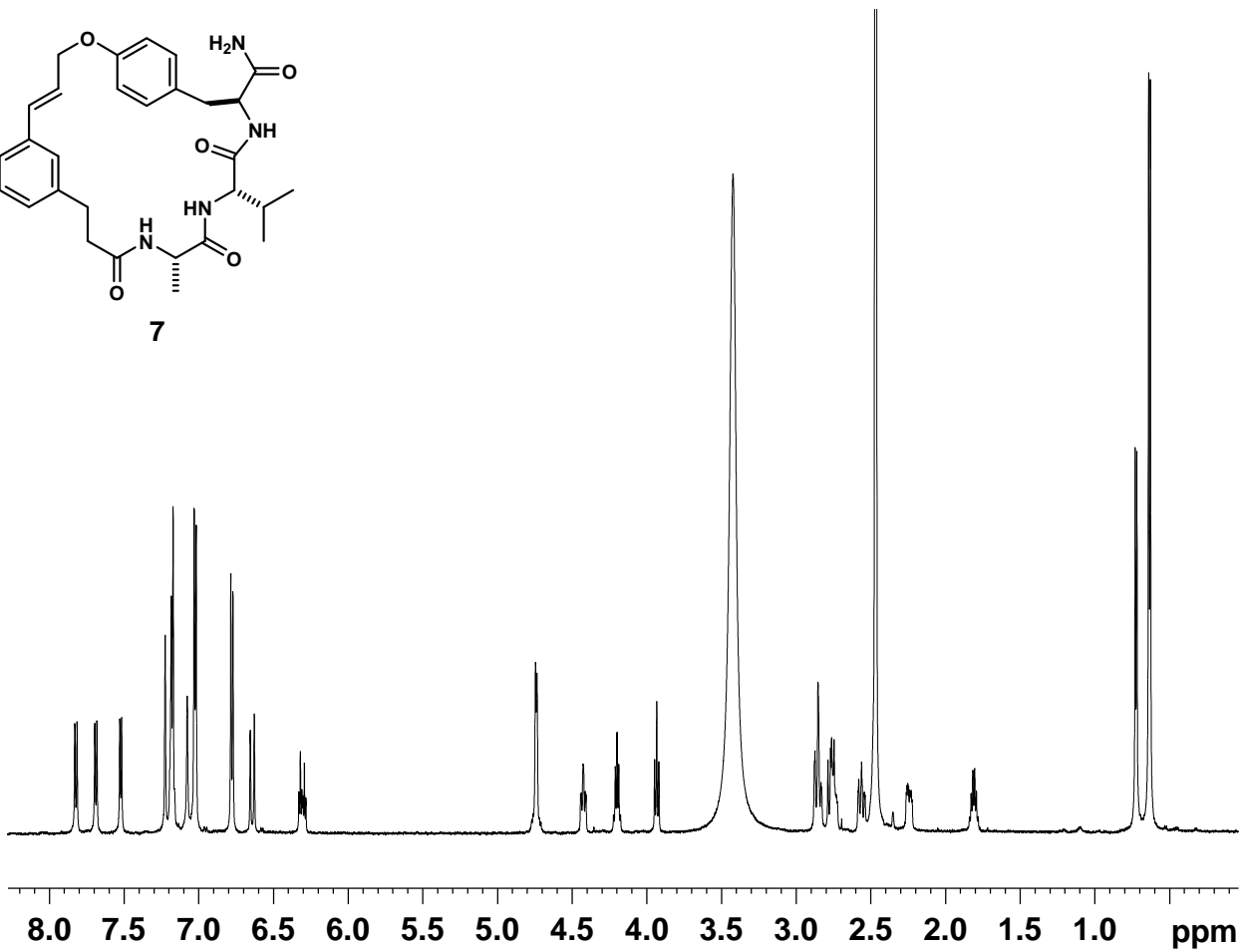
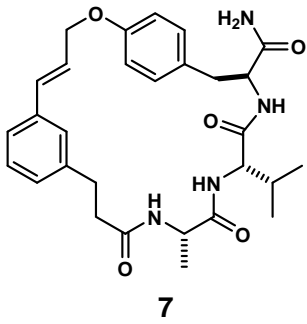
F2 - Acquisition Parameters
Date_         20130518
Time          3.28
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            8192
DS            2
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG            202.91
DW            16.000 usec
DE            18.00 usec
TE            298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          125.7722511 MHz
NUC1          13C
P1            9.63 usec
PLW1          23.00000000 W

===== CHANNEL f2 =====
SFO2          500.1330008 MHz
NUC2          1H
CPDPRG[2]    waltz16
PCPD2         80.00 usec
PLW2          13.50000000 W
PLW12         0.21094000 W
PLW13         0.13500001 W

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00
    
```

Cyclic-Ala-Val-Tyr (7):



```

Current Data Parameters
NAME          KL-4-22
EXPNO         1
PROCNO        1

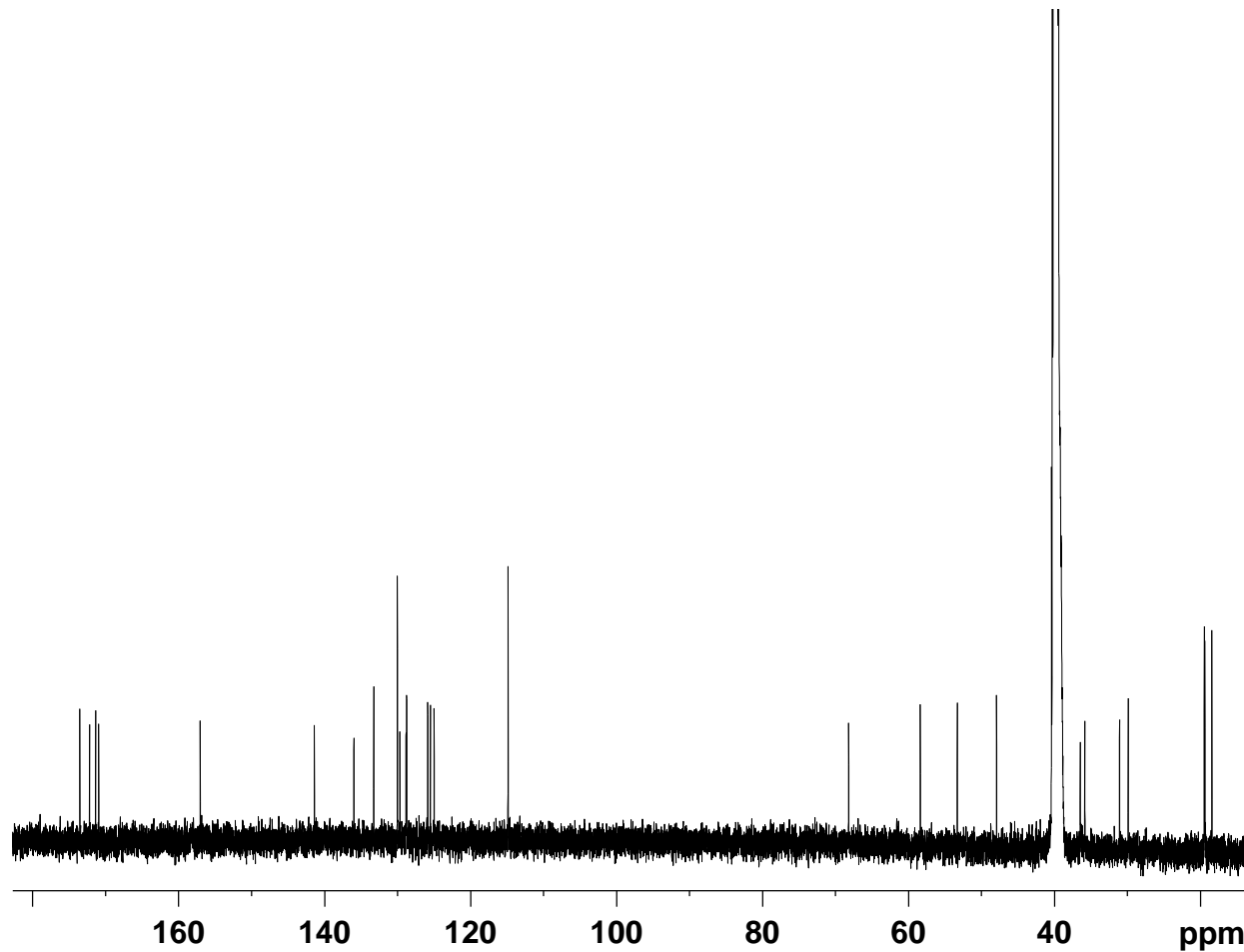
F2 - Acquisition Parameters
Date_         20110926
Time          17.07
INSTRUM       av600
PROBHD        5 mm TBI5
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           12376.237 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            181
DW            40.400 usec
DE            6.50 usec
TE            294.0 K
D1            2.0000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.10 usec
PL1           -2.00 dB
PL1W          39.81071854 W
SFO1          600.1336008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            600.1300273 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



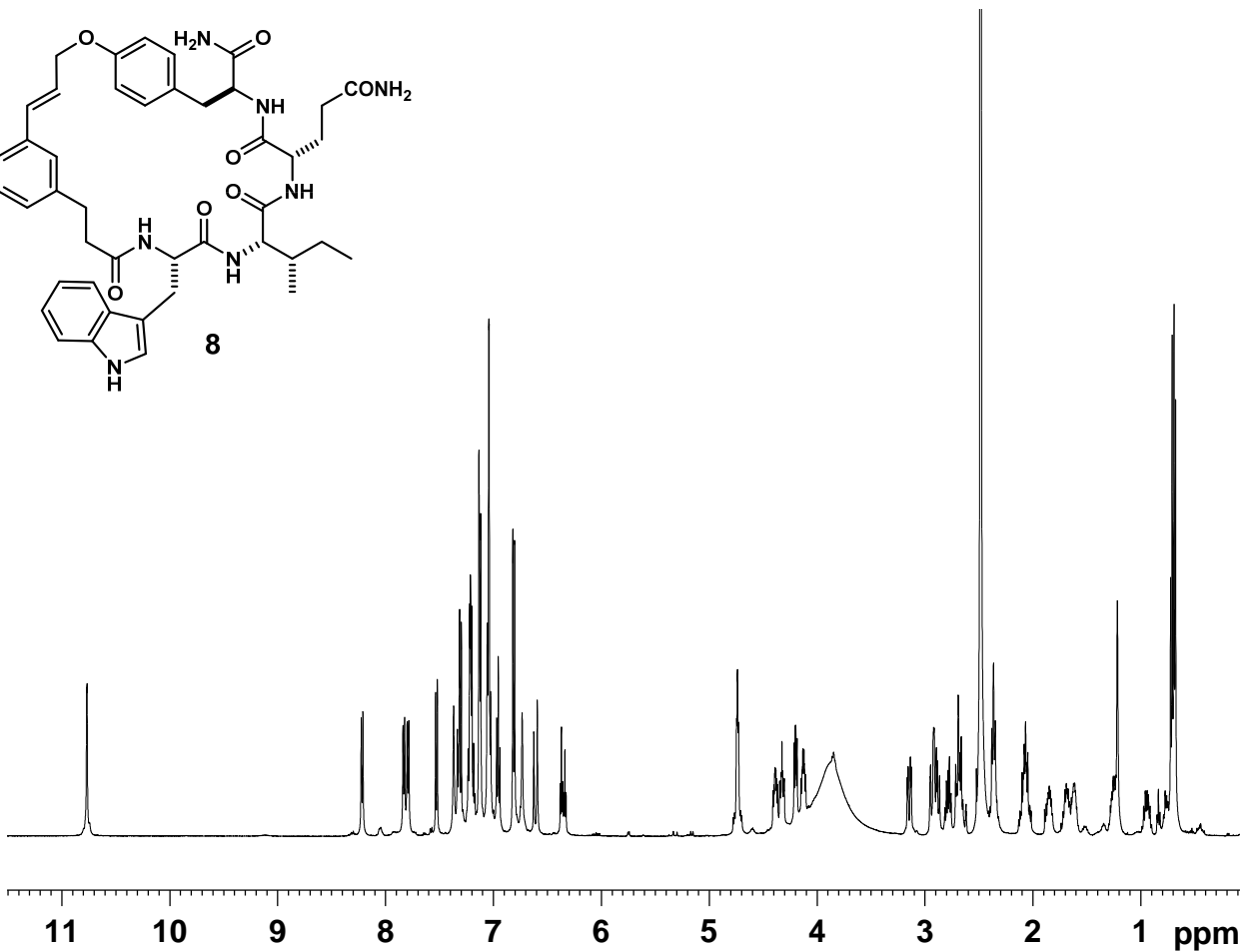
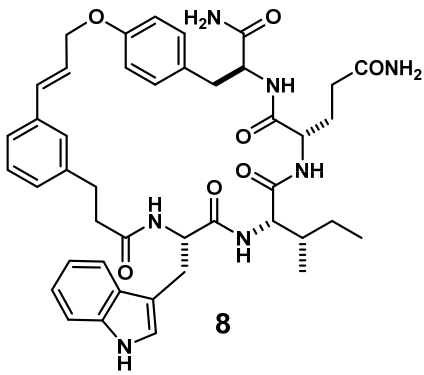
```

Current Data Parameters
NAME          KL-4-22
EXPNO         3
PROCNO        1
    
```

```

F2 - Processing parameters
SI            65536
SF            150.9028319 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

Cyclic-Trp-Ile-Gln-Tyr (8):



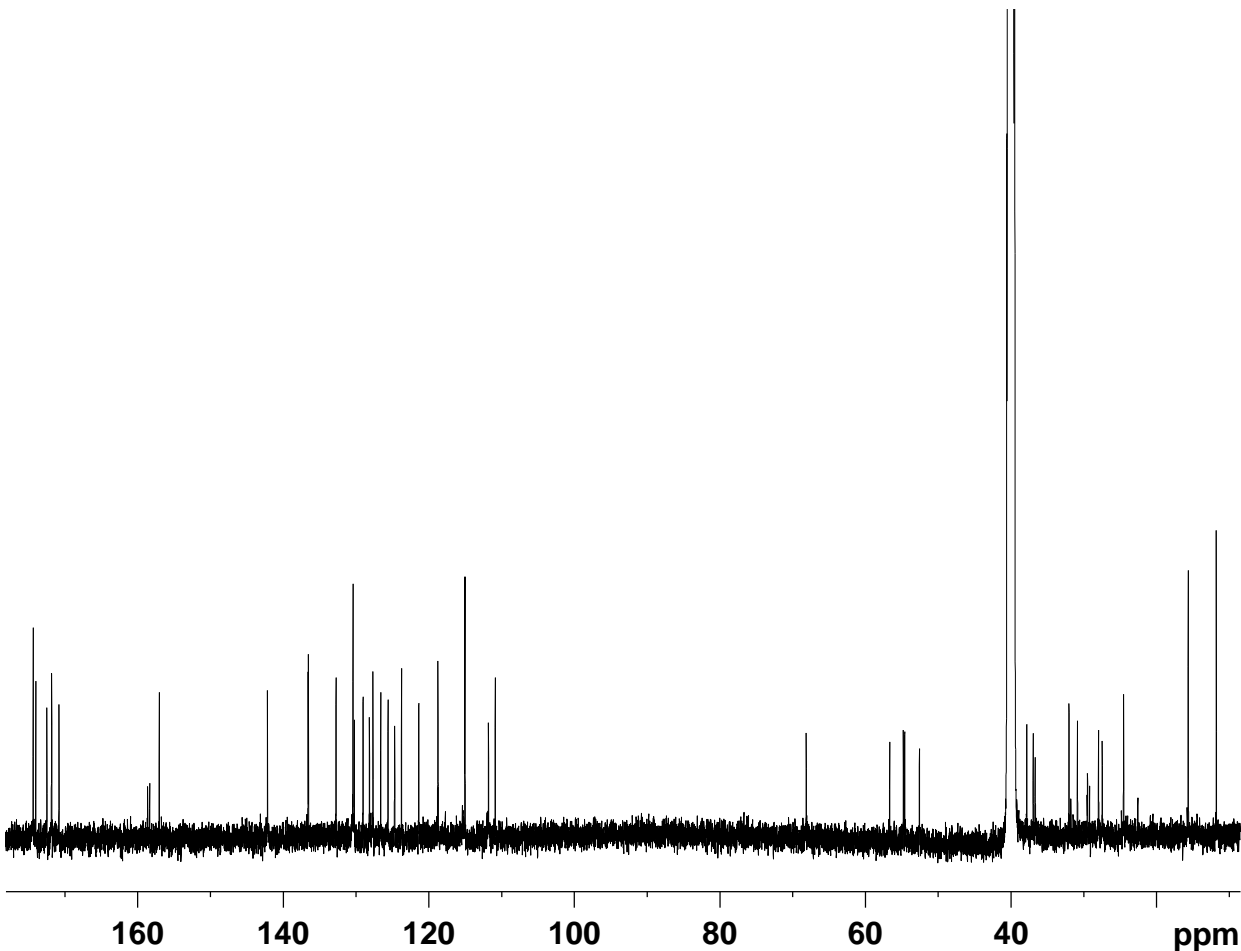
```

Current Data Parameters
NAME          KL-5-117b
EXPNO         3
PROCNO        1

F2 - Acquisition Parameters
Date_         20130204
Time          18.16
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            64
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            11
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
DL            2.0000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          500.1330008 MHz
NUC1           1H
P1            10.00 usec
PLW1          13.5000000 W

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```



```

Current Data Parameters
NAME          KL-5-117b
EXPNO         4
PROCNO        1

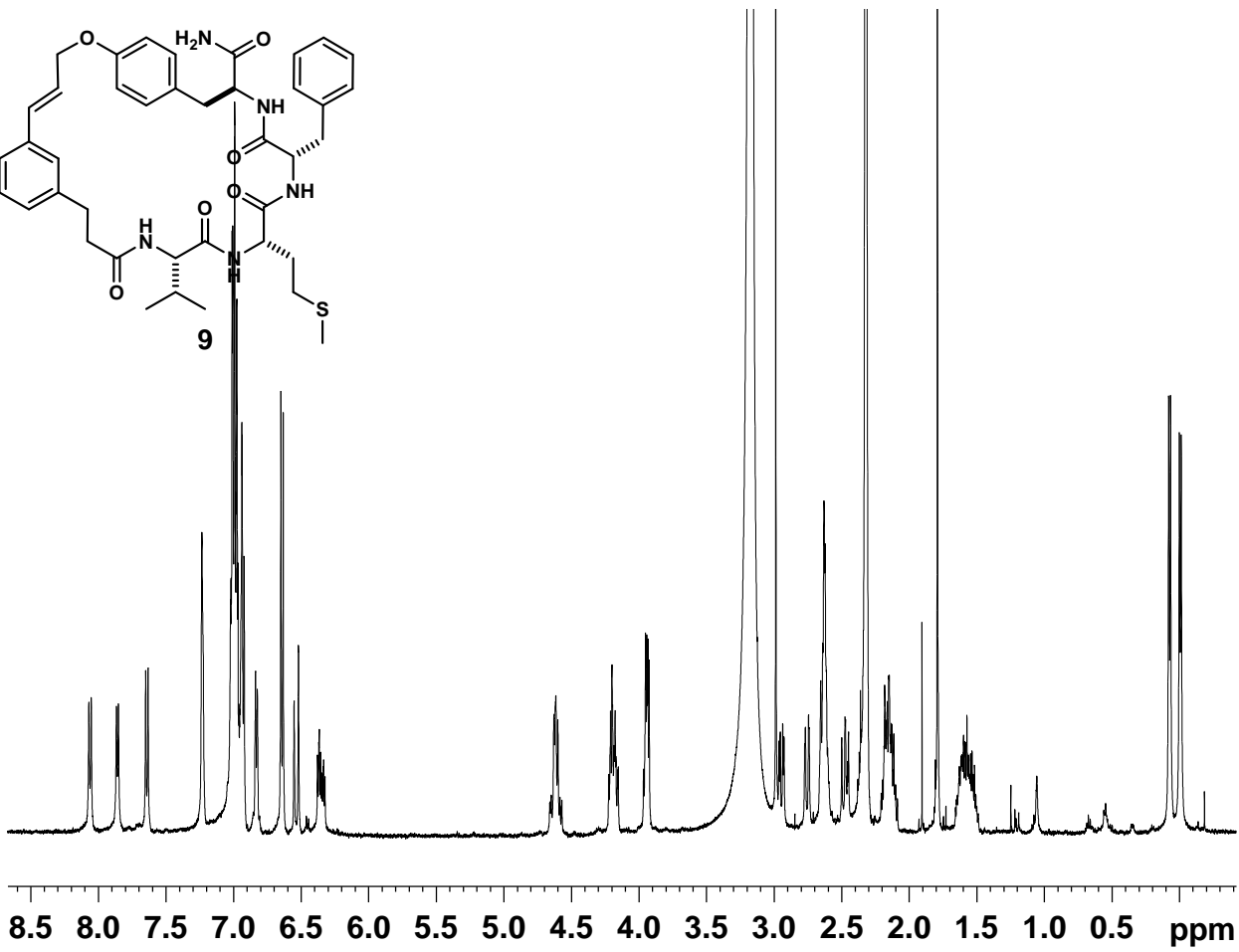
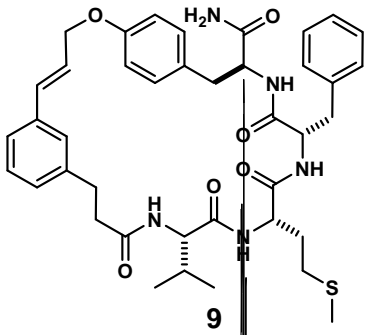
F2 - Acquisition Parameters
Date_         20130204
Time          19.00
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            861
DS            2
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG            202.91
DW            16.000 usec
DE            18.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          125.7722511 MHz
NUC1           13C
P1             9.63 usec
PLW1          23.0000000 W

===== CHANNEL f2 =====
SFO2          500.1330008 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          13.5000000 W
PLW12         0.21094000 W
PLW13         0.13500001 W

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```


Cyclic-Val-Met-Phe-Tyr (9):



```

Current Data Parameters
NAME      KL-4-56_ICON
EXPNO    1
PROCNO   1

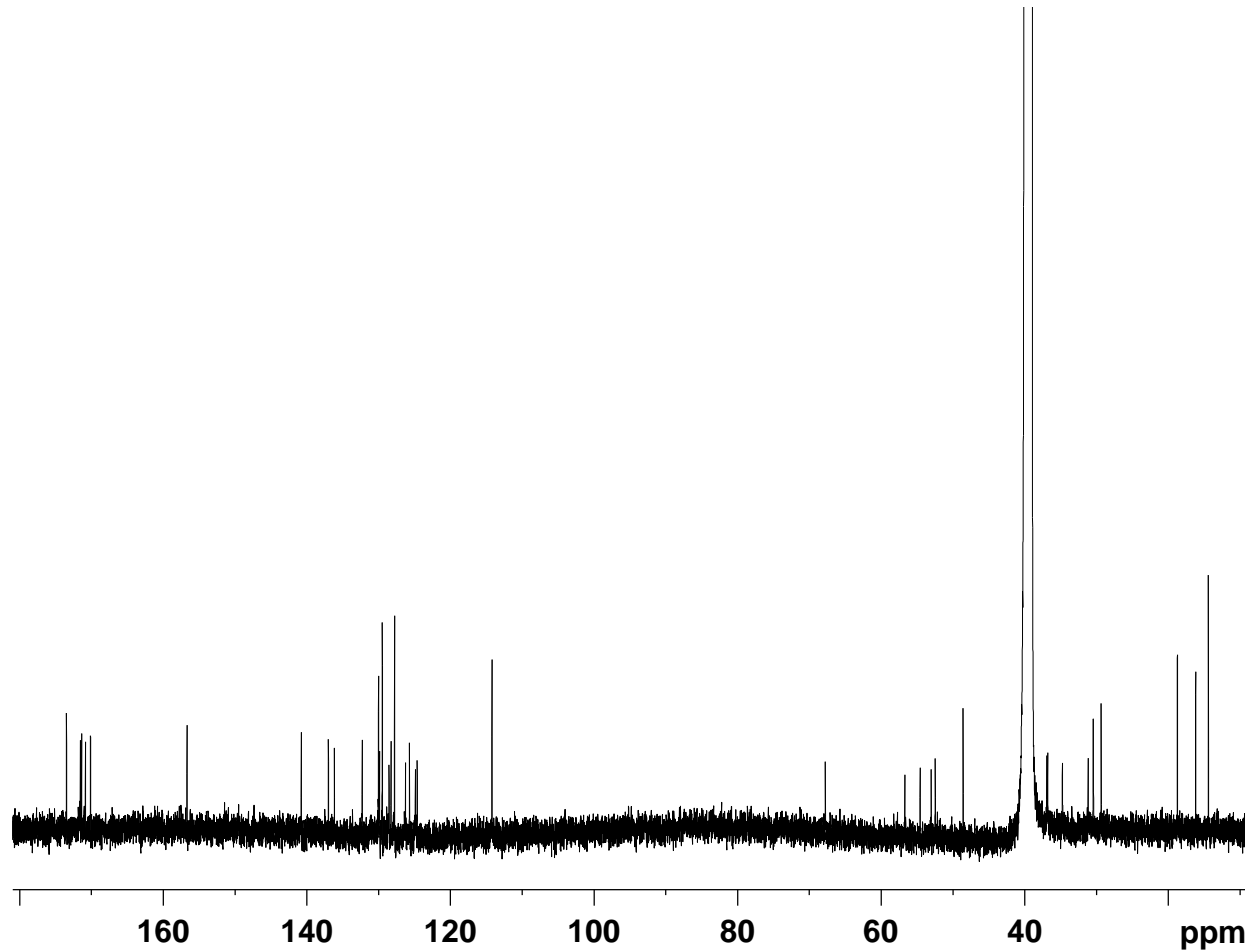
F2 - Acquisition Parameters
Date_    20120827
Time     22.07
INSTRUM  av500
PROBHD   5 mm DCH 13C-1
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       28.6
DW       50.000 usec
DE       10.00 usec
TE       298.0 K
D1       2.00000000 sec
TD0      1
    
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       10.00 usec
PLW1    13.5000000 W
SFO1    500.1330008 MHz
    
```

```

F2 - Processing parameters
SI       65536
SF       500.1300950 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



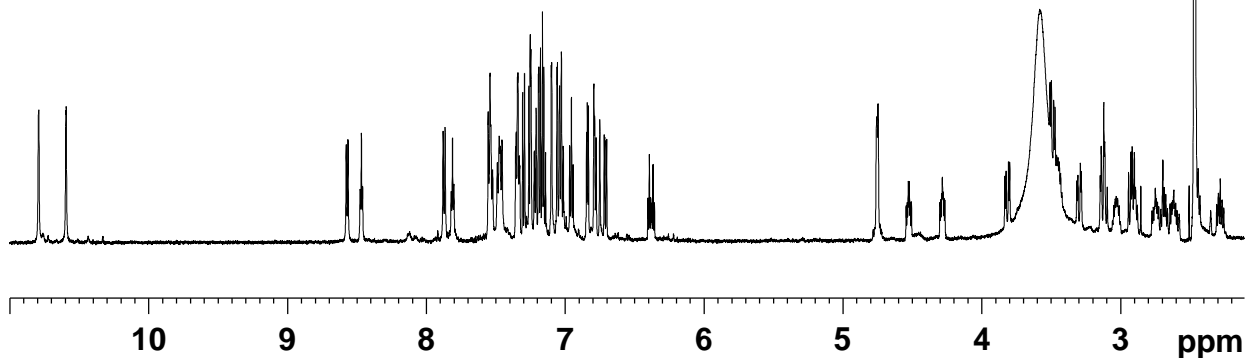
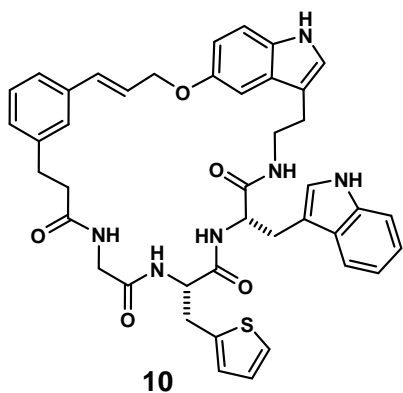
```

Current Data Parameters
NAME      KL-4-56_ICON
EXPNO    2
PROCNO   1
    
```

```

F2 - Processing parameters
SI       131072
SF       125.7578519 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

Cyclic-Gly-Thi-Trp-5HT (10):

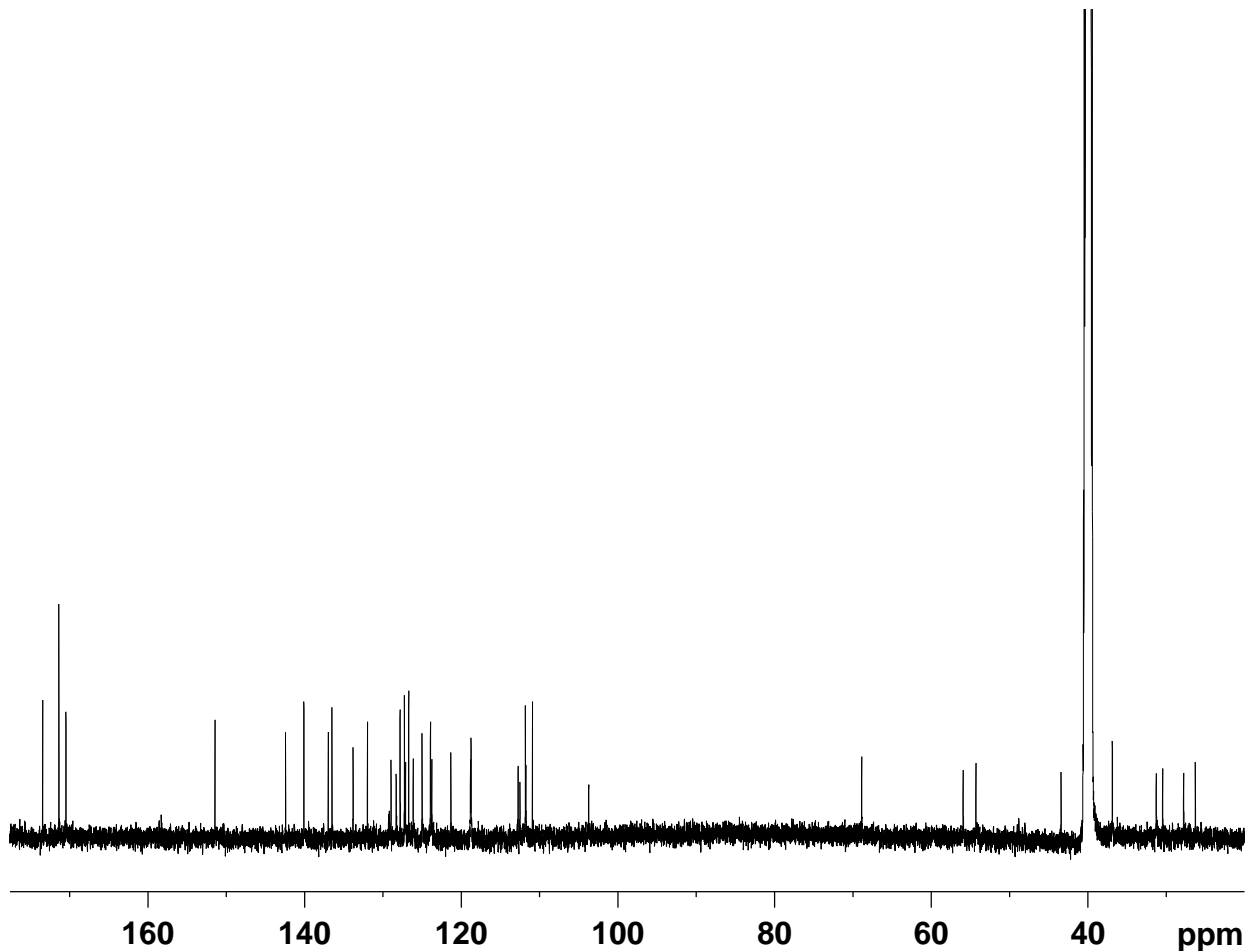


```
Current Data Parameters
NAME      KL-4-171B
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20120409
Time     19.19
INSTRUM av600
PROBHD   5 mm TBI5
PULPROG zg30
TD       65536
SOLVENT  DMSO
NS       8
DS       0
SWH      12376.237 Hz
FIDRES   0.188846 Hz
AQ       2.6476543 sec
RG       181
DW       40.400 usec
DE       6.50 usec
TE       294.6 K
D1       2.0000000 sec
TD0     1
```

```
===== CHANNEL f1 =====
NUC1     1H
P1       9.10 usec
PL1     -2.00 dB
PL1W    39.81071854 W
SFO1    600.1336008 MHz
```

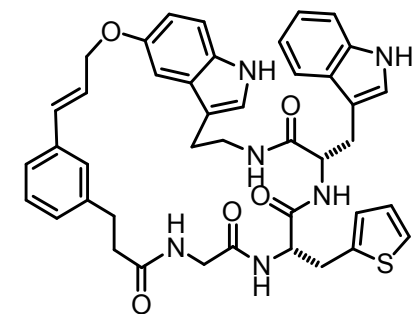
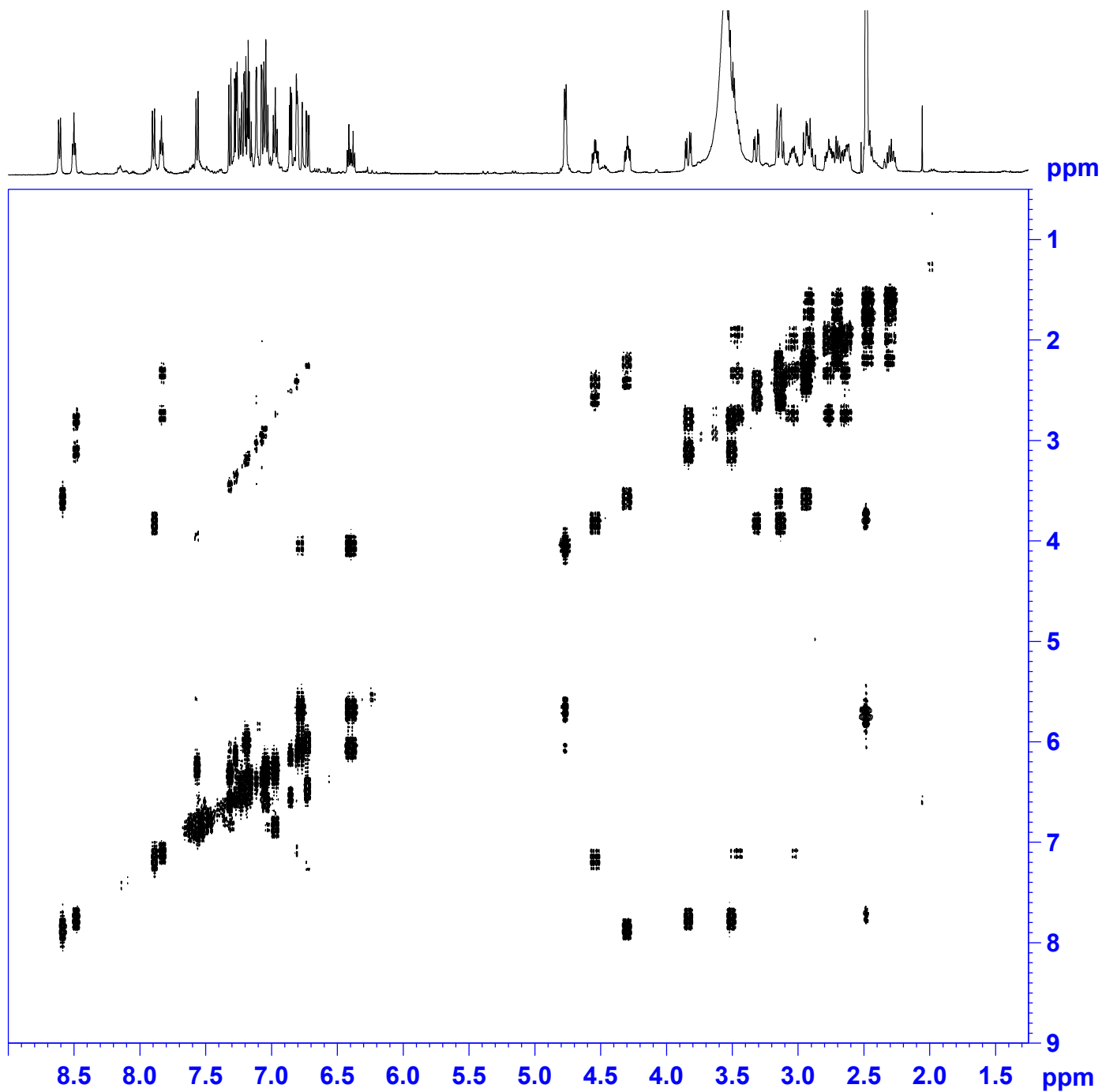
```
F2 - Processing parameters
SI       65536
SF       600.1300273 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
```



```
Current Data Parameters
NAME      KL-4-171A_500A
EXPNO    2
PROCNO   1
```

```
F2 - Acquisition Parameters
Date_    20120411
Time     18.26
INSTRUM av500
PROBHD   5 mm DCH 13C-1
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       600
DS       2
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0485760 sec
RG       202.91
DW       16.000 usec
DE       18.00 usec
TE       296.0 K
D1       2.0000000 sec
d11     0.03000000 sec
DELTA    1.89999998 sec
TD0     1
SFO1    125.7722511 MHz
NUC1    13C
P1       9.63 usec
PLW1    23.00000000 W
SFO2    500.1330008 MHz
NUC2    1H
CPDPRG[2] waltz16
PCPD2   80.00 usec
PLW2    13.50000000 W
PLW12   0.21094000 W
PLW13   0.13500001 W
```

```
F2 - Processing parameters
SI       131072
SF       125.7577892 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```



Current Data Parameters

NAME KL-4-171A_500A
 EXPNO 5
 PROCNO 1

F1 - Acquisition parameters

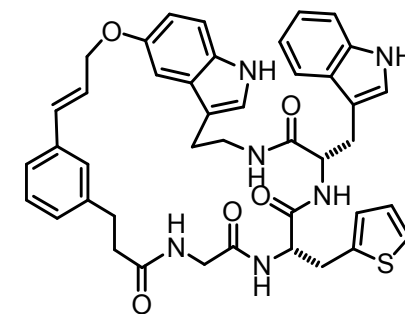
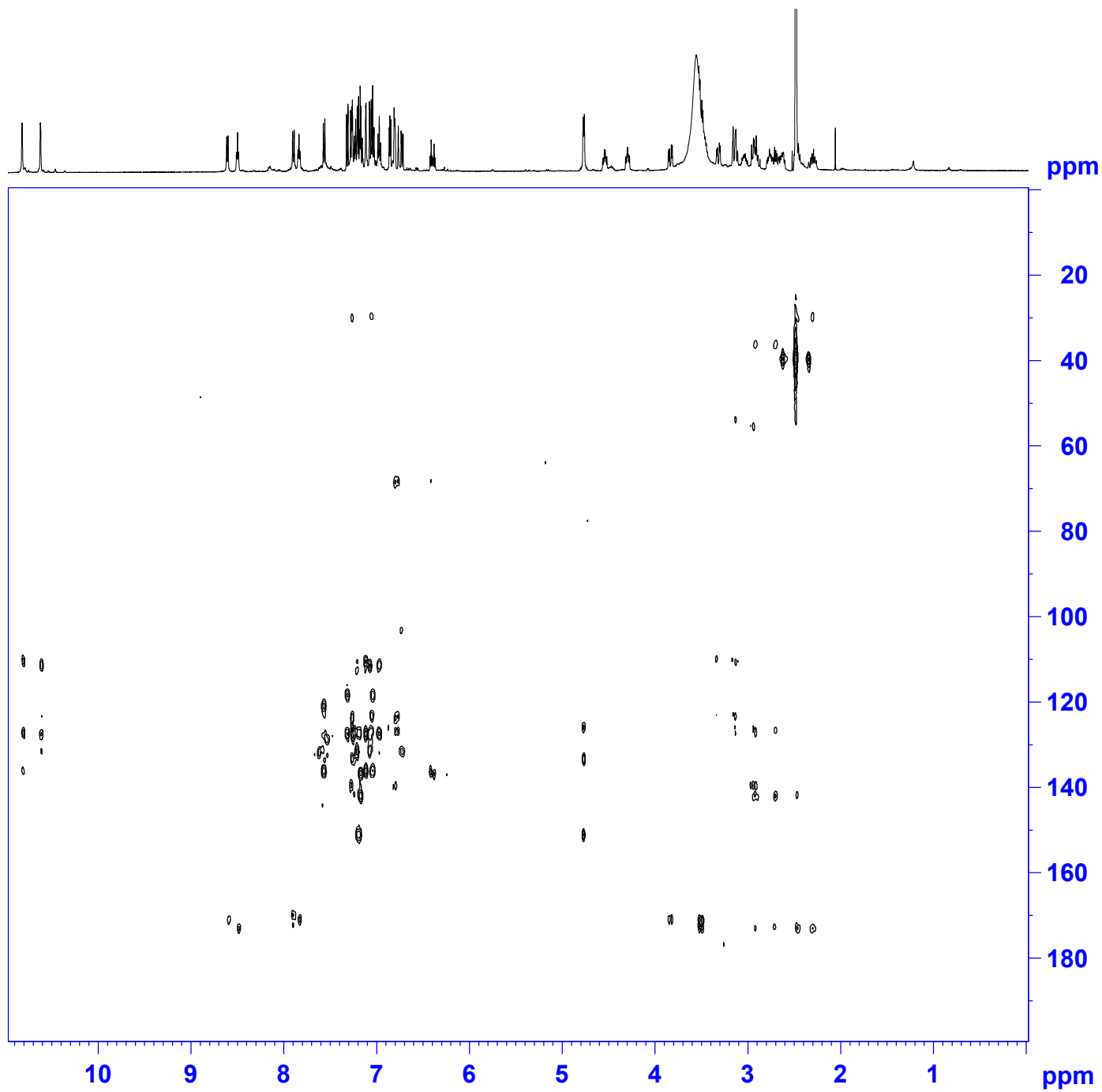
TD 256
 SFO1 500.1328 MHz
 FIDRES 19.536423 Hz
 SW 10.000 ppm
 FnmODE States-TPPI

F2 - Processing parameters

SI 2048
 SF 500.1300135 MHz
 WDW SINE
 SSB 1
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters

SI 2048
 MC2 States-TPPI
 SF 500.1303720 MHz
 WDW QSINE
 SSB 1
 LB 0 Hz
 GB 0



Current Data Parameters

NAME KL-4-171A_500A
 EXPNO 6
 PROCNO 1

F1 - Acquisition parameters

TD 162
 SFO1 125.7704 MHz
 FIDRES 155.271286 Hz
 SW 199.999 ppm
 FnmODE QF

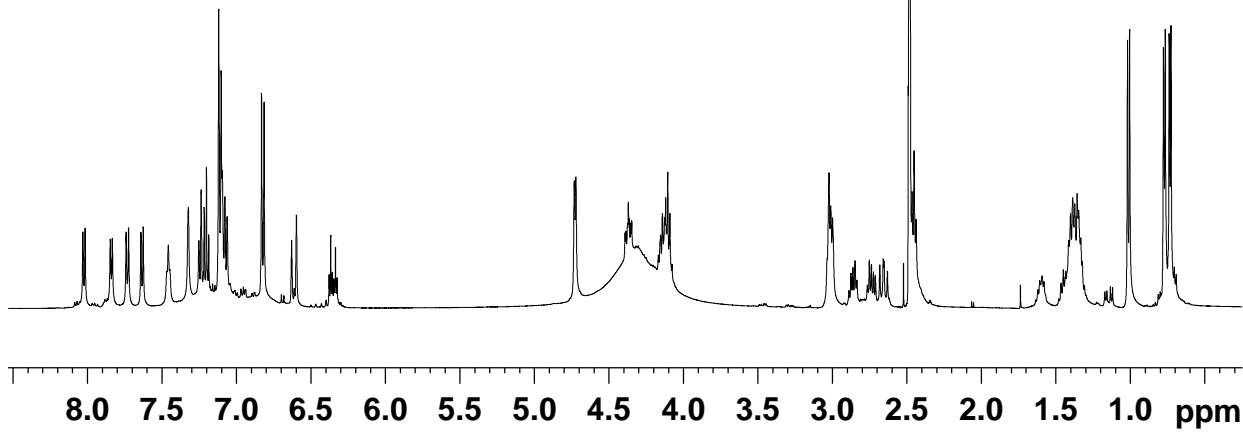
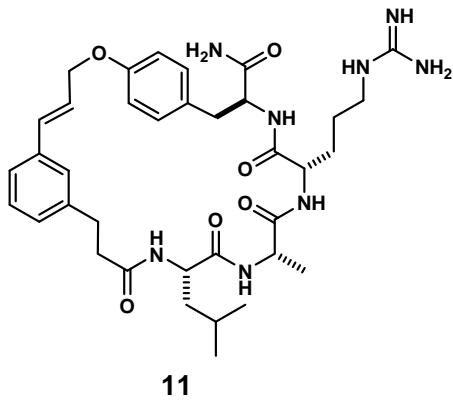
F2 - Processing parameters

SI 2048
 SF 500.1300135 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters

SI 2048
 MC2 QF
 SF 125.7578472 MHz
 WDW
 SSB 2
 LB 0 Hz
 GB 0

Cyclic- Leu-Ala-Arg-Tyr (11):



```

Current Data Parameters
NAME      KL-4-51_CHECK
EXPNO     1
PROCNO    1

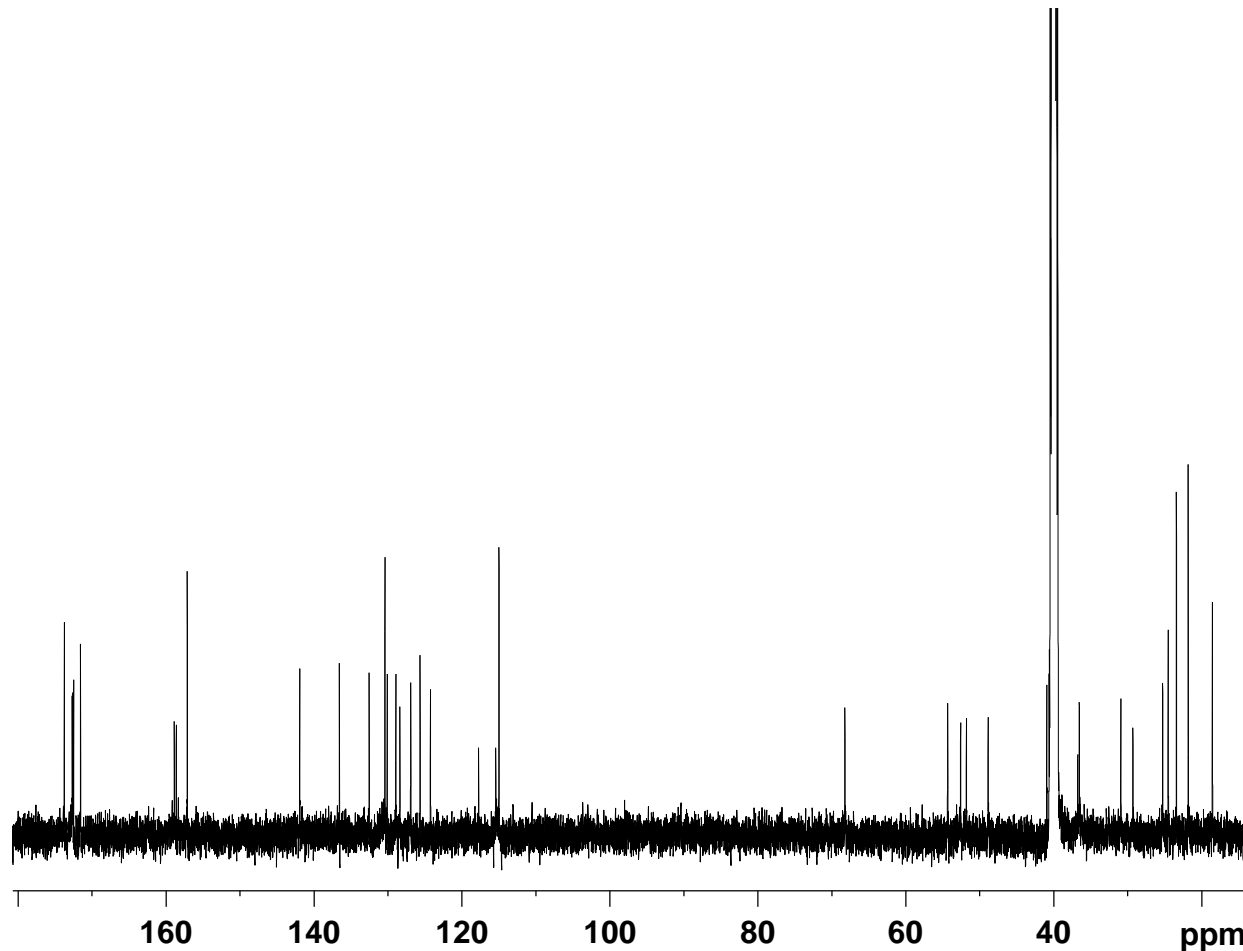
F2 - Acquisition Parameters
Date_     20111019
Time      19.37
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2767999 sec
RG         22.82
DW         50.000 usec
DE         10.00 usec
TE         301.0 K
D1         2.0000000 sec
TD0        1
    
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
PLW1      13.5000000 W
SF01      500.1330008 MHz
    
```

```

F2 - Processing parameters
SI         65536
SF         500.1300146 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

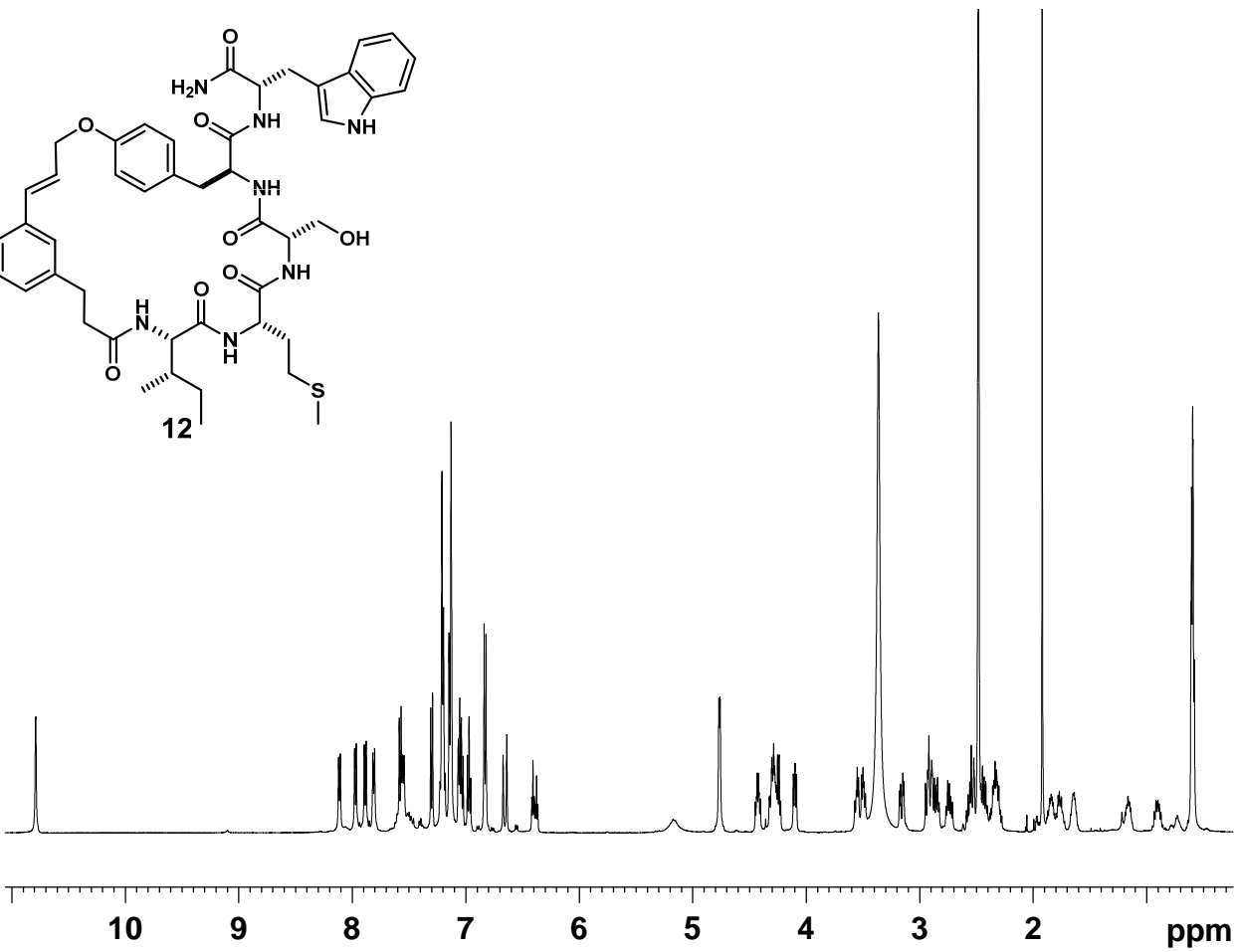
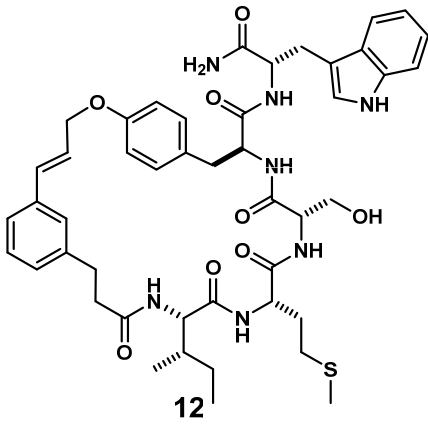


```

Current Data Parameters
NAME      KL-4-51_CHECK
EXPNO     2
PROCNO    1

F2 - Processing parameters
SI         131072
SF         125.7577892 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
    
```

Cyclic-Ile-Met-Ser-Tyr-Trp (12):



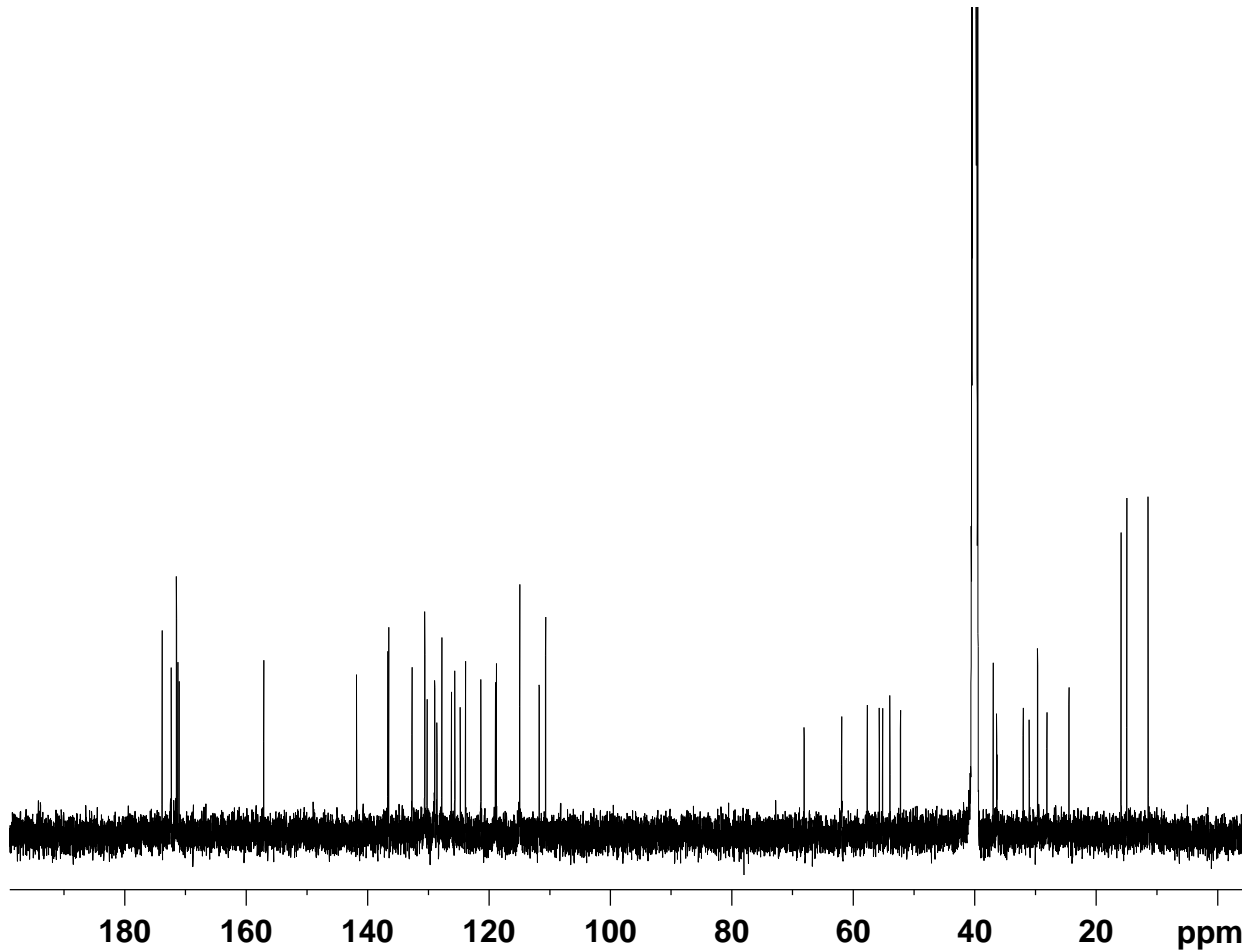
```

Current Data Parameters
NAME          KL-4-57
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20111019
Time          19.25
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            20.17
DW            50.000 usec
DE            10.00 usec
TE            301.0 K
D1            2.0000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            10.00 usec
PLW1         13.5000000 W
SF01         500.1330008 MHz

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

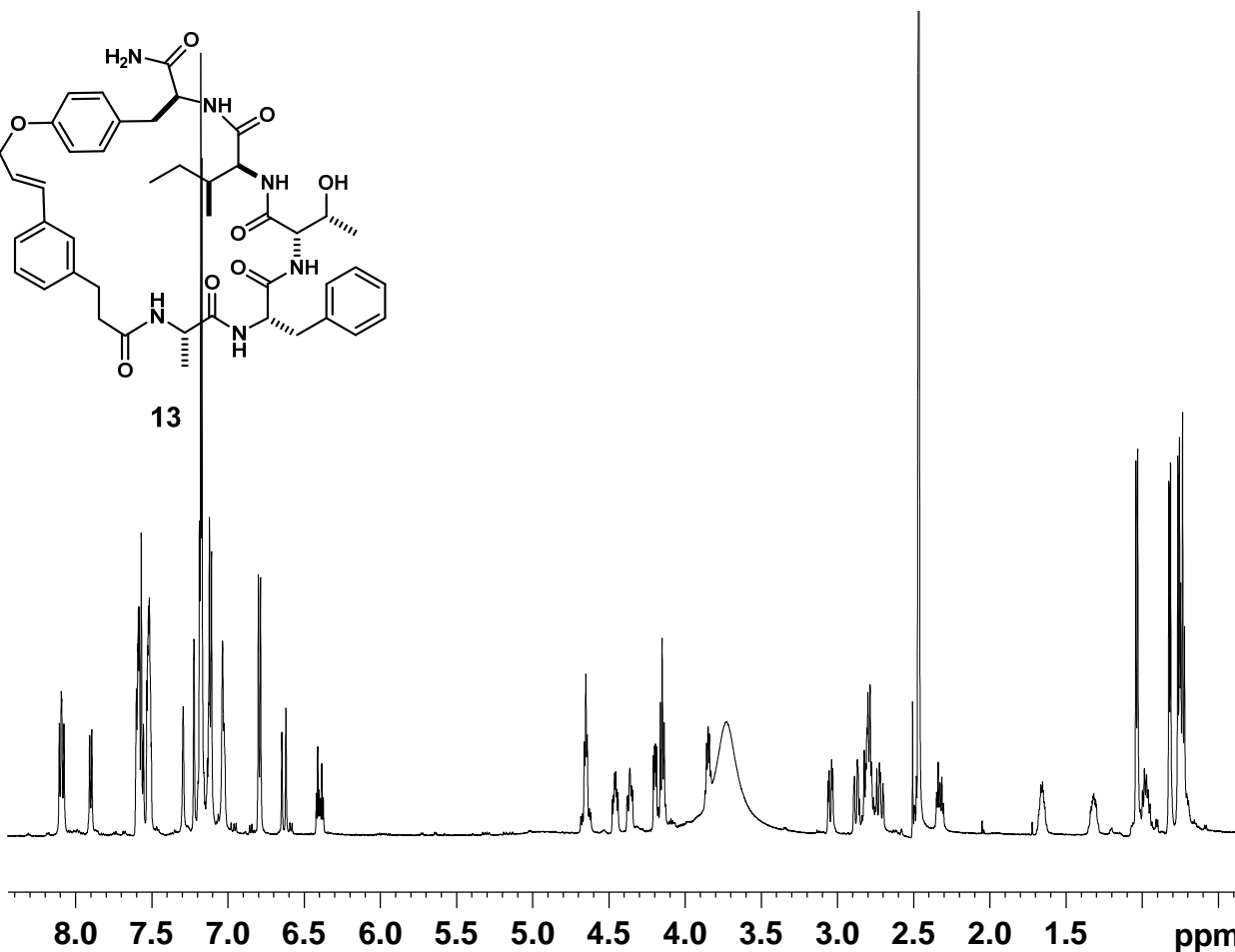
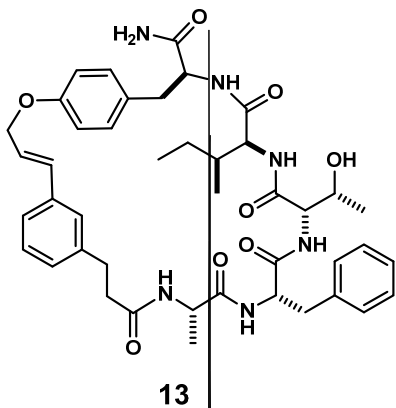


```

Current Data Parameters
NAME          KL-4-57
EXPNO         2
PROCNO        1

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

Cyclic- Ala-Phe-Thr-Ile-Tyr (13):



```

Current Data Parameters
NAME          KL-4-48
EXPNO         1
PROCNO        1

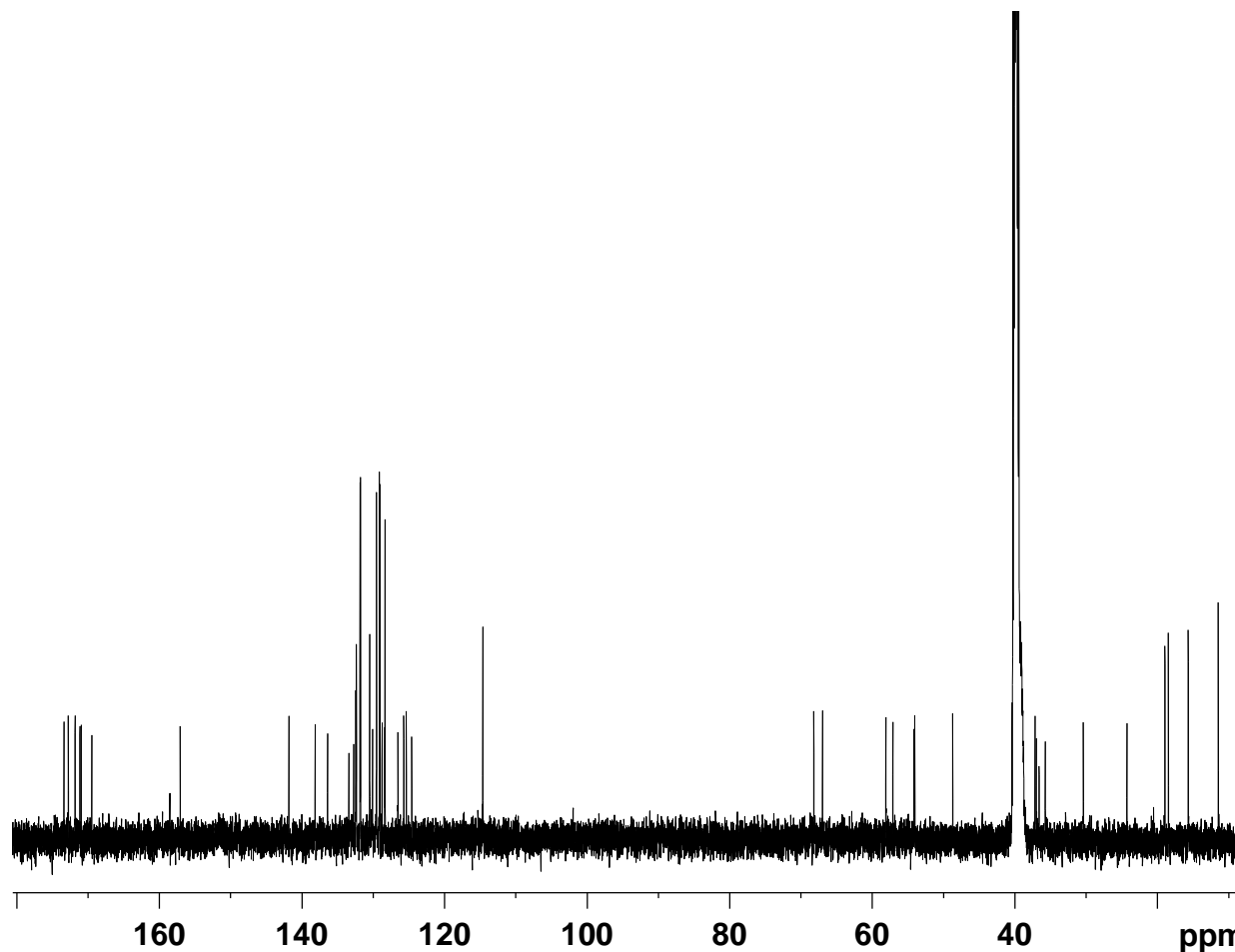
F2 - Acquisition Parameters
Date_         20111007
Time          10.20
INSTRUM       av600
PROBHD        5 mm TBI5
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           12376.237 Hz
FIDRES        0.188846 Hz
AQ            2.6476543 sec
RG            181
DW            40.400 usec
DE            6.50 usec
TE            295.8 K
D1            2.0000000 sec
TD0           1
    
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.10 usec
PL1           -2.00 dB
PL1W          39.81071854 W
SFO1          600.1336008 MHz
    
```

```

F2 - Processing parameters
SI            65536
SF            600.1300273 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

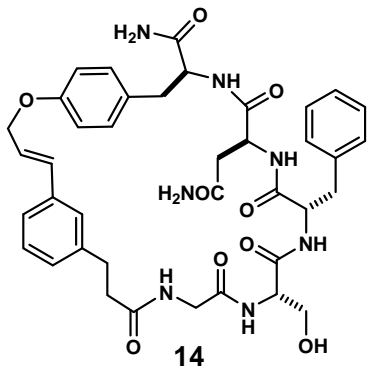


```

Current Data Parameters
NAME          KL-4-48
EXPNO         3
PROCNO        1

F2 - Processing parameters
SI            65536
SF            150.9028319 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

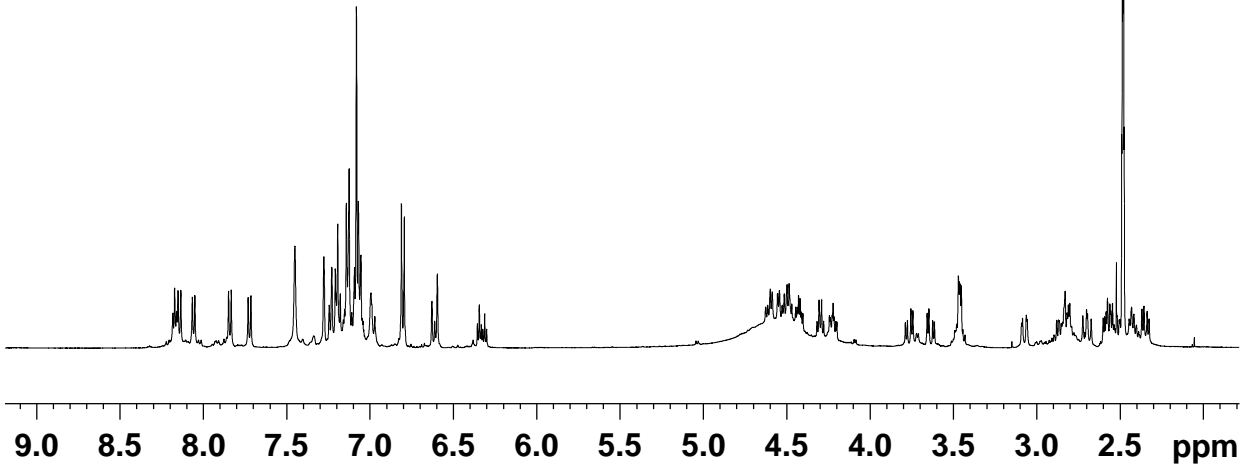
Cyclic-Gly-Ser-Phe-Asn-Tyr (14):



```

Current Data Parameters
NAME          KL-4-58
EXPNO         1
PROCNO        1

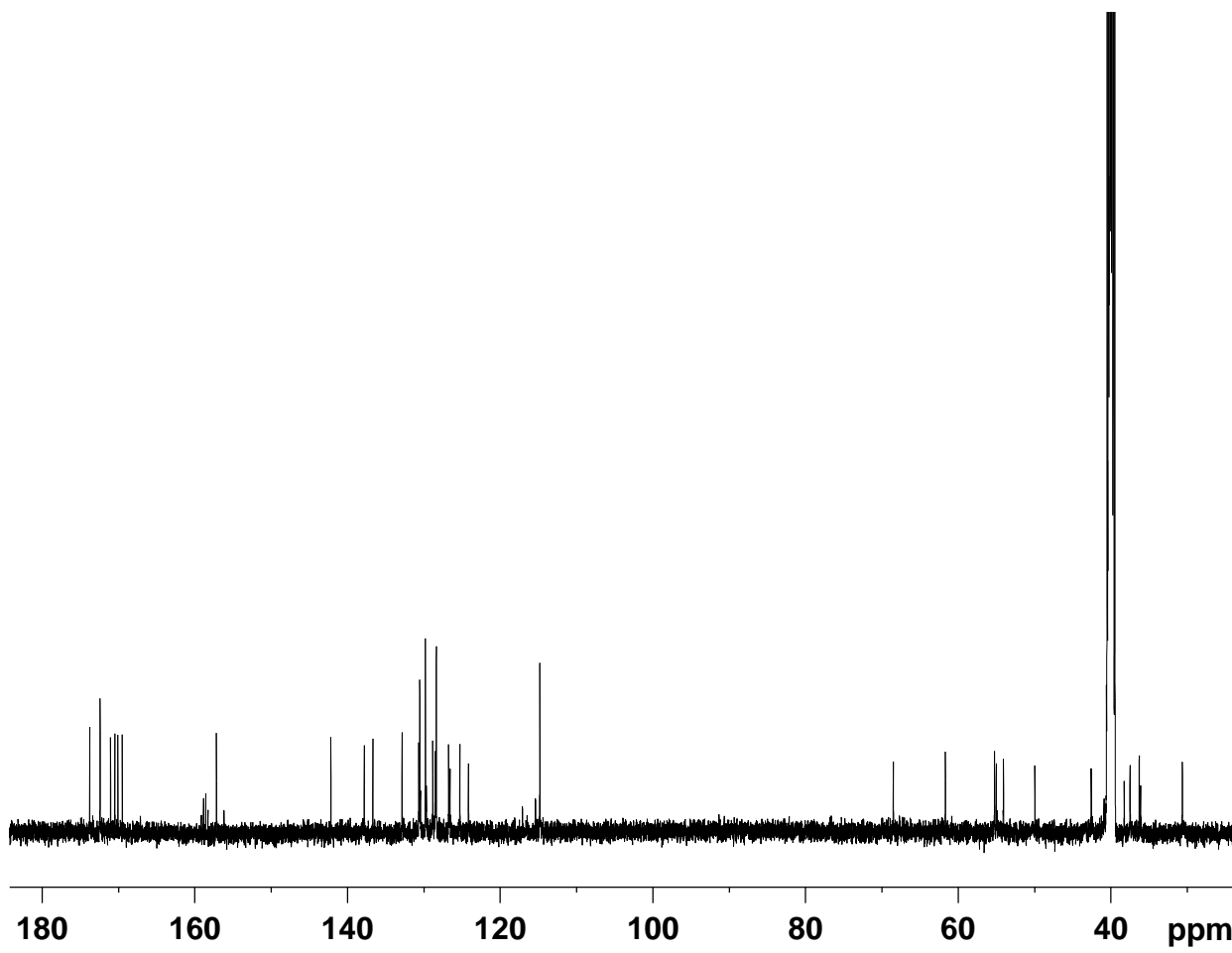
F2 - Acquisition Parameters
Date_         20111019
Time          19.11
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD             65536
SOLVENT       DMSO
NS             4
DS             0
SWH            10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG             60.32
DW             50.000 usec
DE             10.00 usec
TE             301.0 K
D1             2.0000000 sec
TD0            1
    
```



```

===== CHANNEL f1 =====
NUC1          1H
P1            10.00 usec
PLW1          13.5000000 W
SF01          500.1330008 MHz

F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

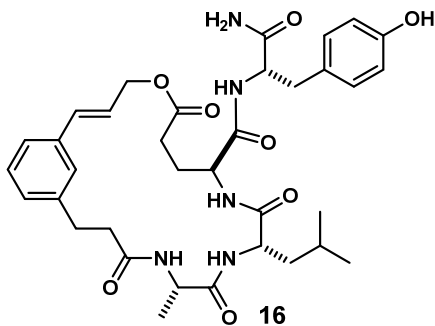


```

Current Data Parameters
NAME          KL-4-58
EXPNO         2
PROCNO        1

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```


Cyclic-Ala-Leu-Glu-Tyr (16):



```

Current Data Parameters
NAME      KL-4-50_f92
EXPNO    1
PROCNO   1

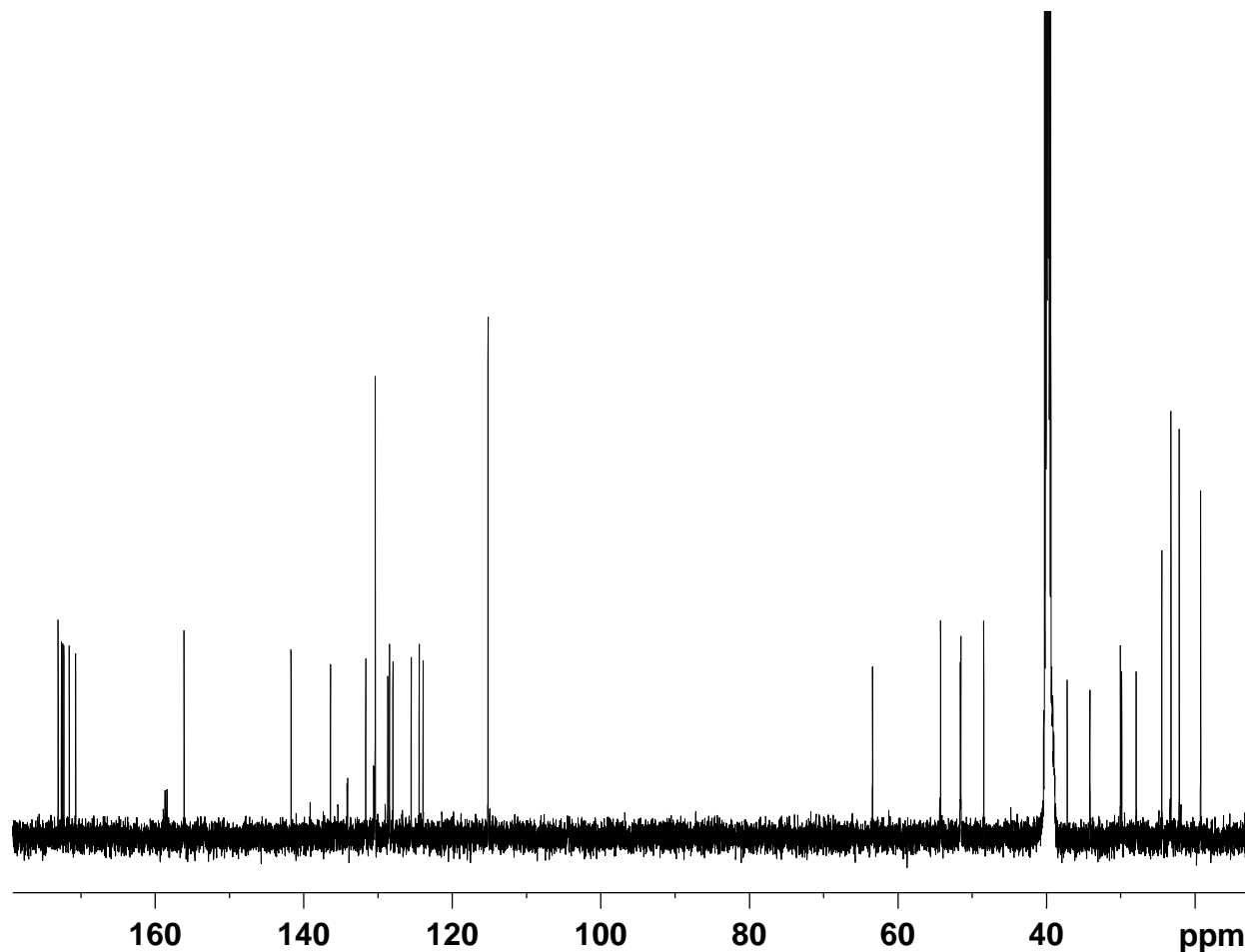
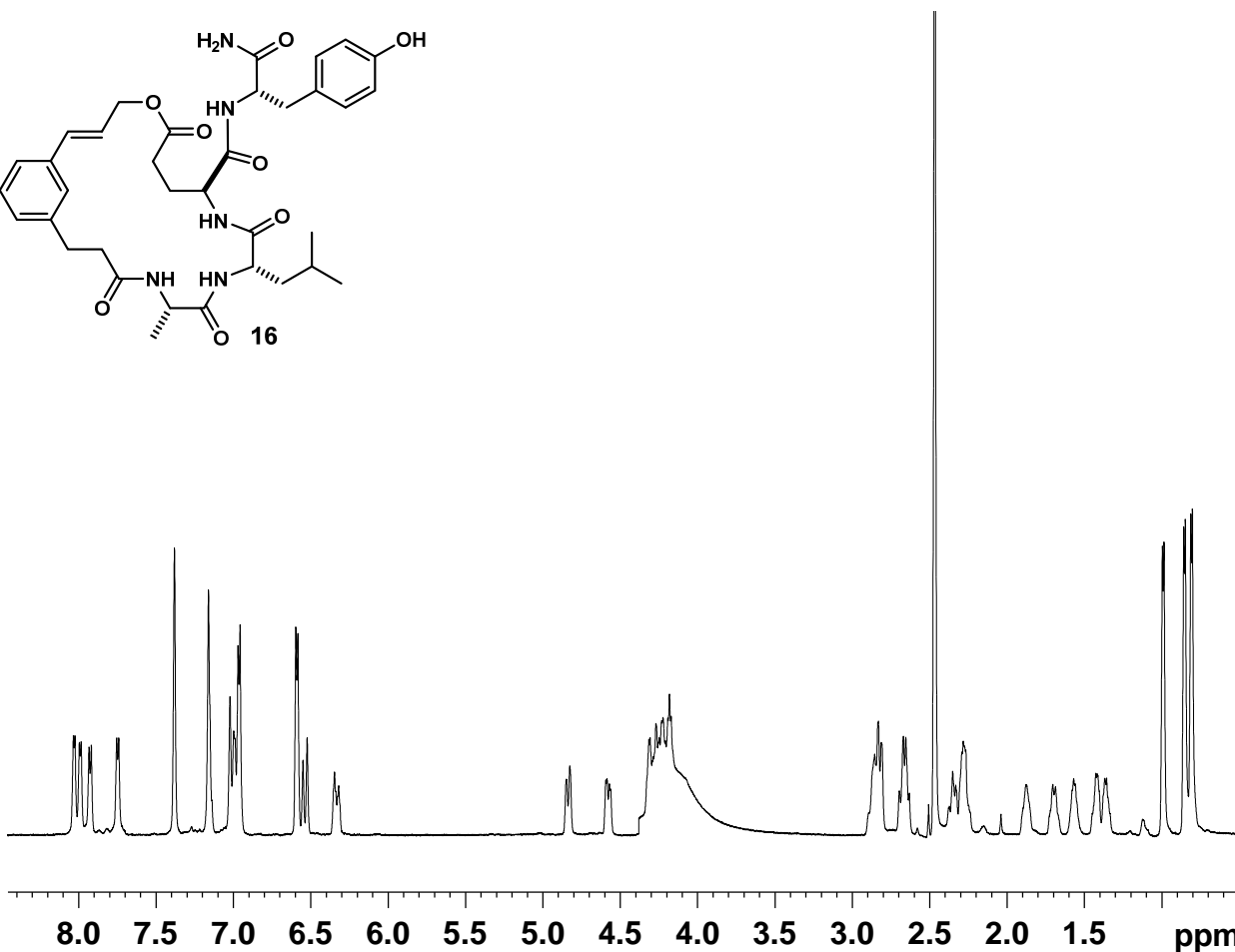
F2 - Acquisition Parameters
Date_    20111008
Time     19.54
INSTRUM  av600
PROBHD   5 mm TBI5
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       8
DS       0
SWH      12376.237 Hz
FIDRES   0.188846 Hz
AQ       2.6476543 sec
RG       181
DW       40.400 usec
DE       6.50 usec
TE       295.7 K
D1       2.0000000 sec
TD0      1
    
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       9.10 usec
PL1      -2.00 dB
PL1W     39.81071854 W
SFO1     600.1336008 MHz
    
```

```

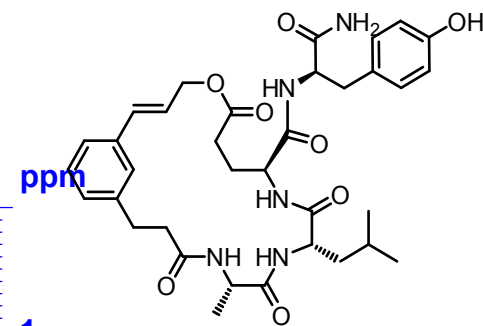
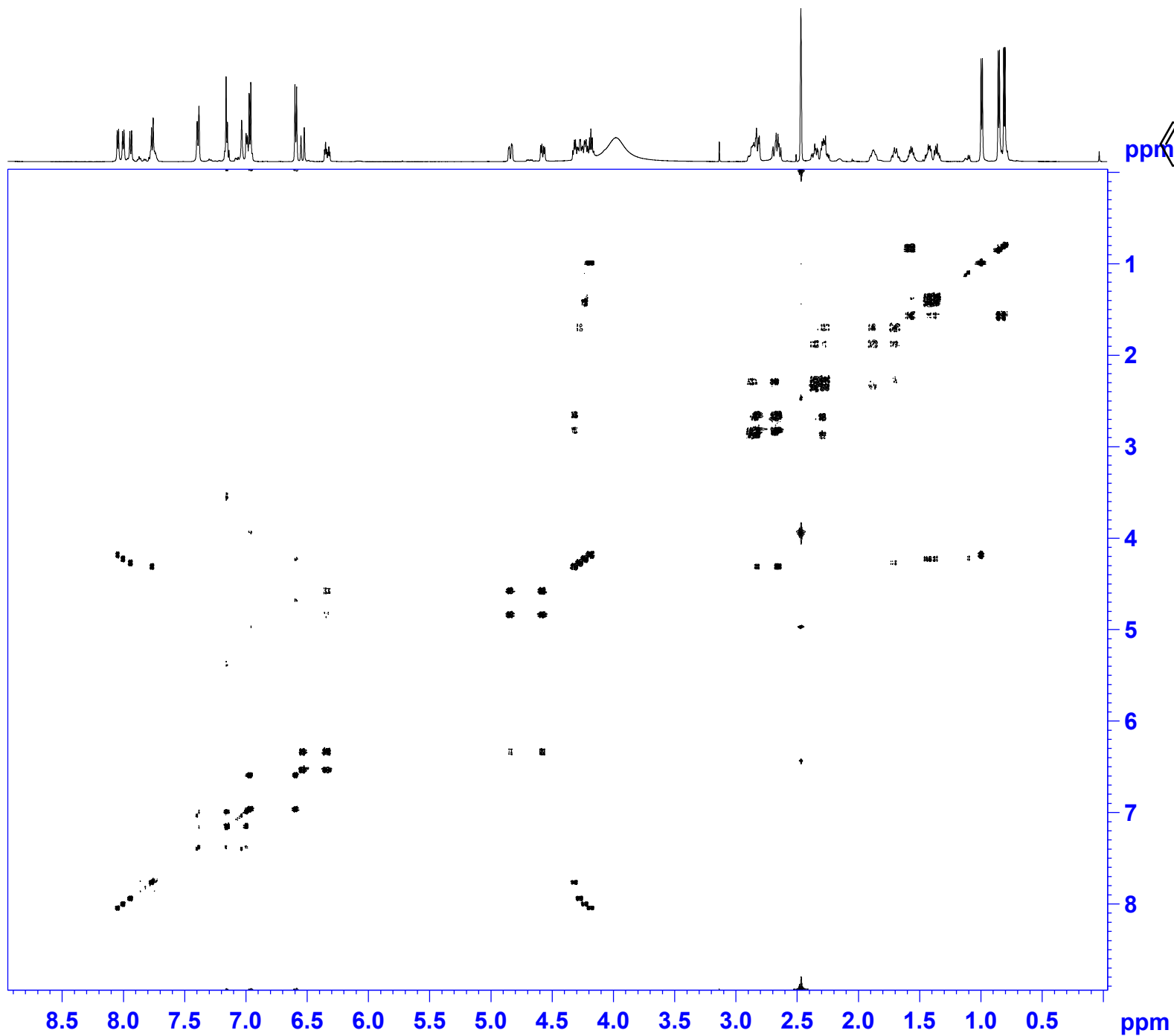
F2 - Processing parameters
SI       65536
SF       600.1300273 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



```

Current Data Parameters
NAME      KL-4-59
EXPNO    7
PROCNO   1

F2 - Processing parameters
SI       65536
SF       150.9028319 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```

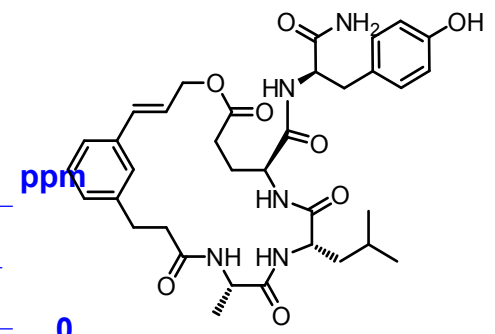
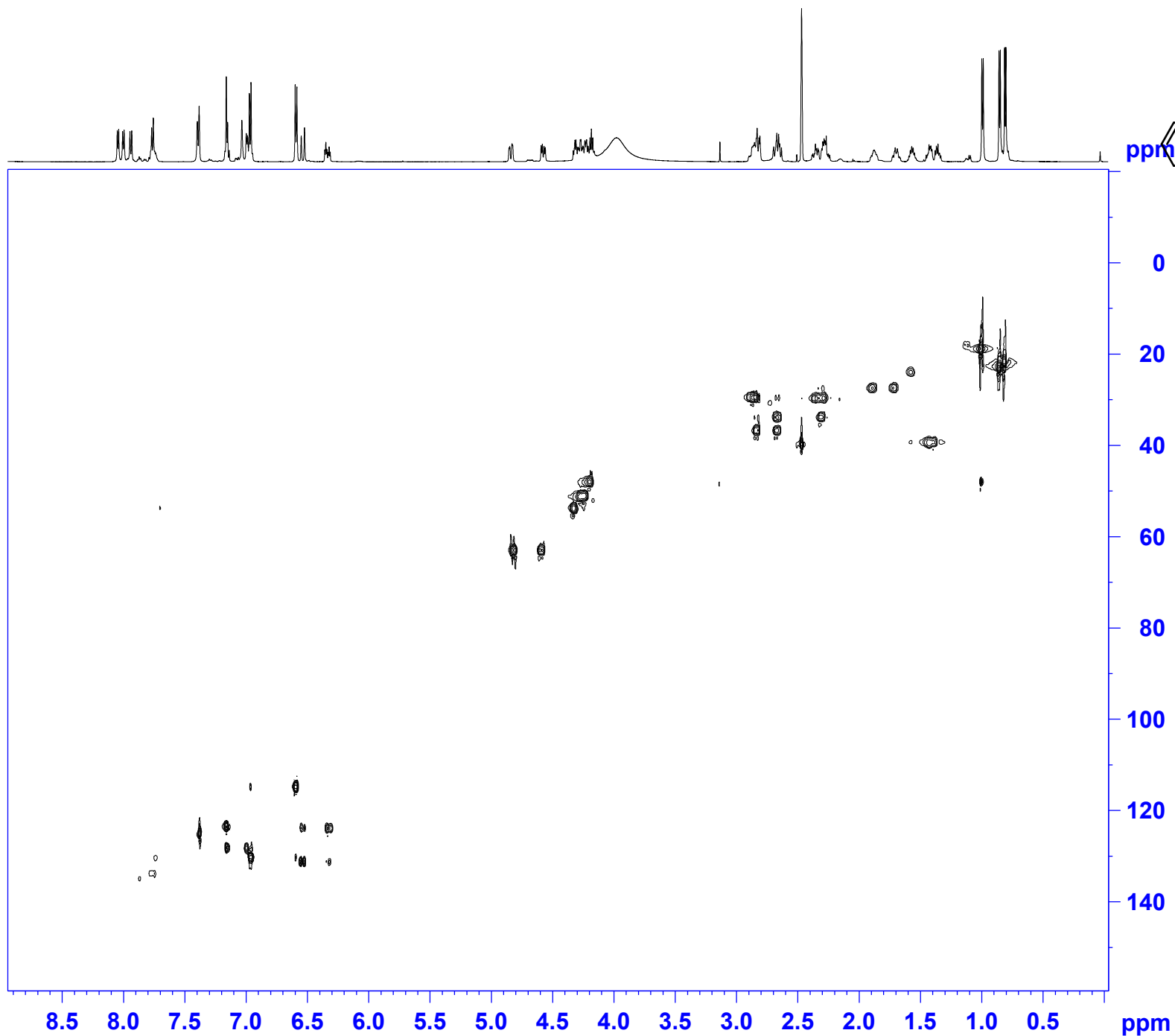


Current Data Parameters
 NAME KL-4-59
 EXPNO 2
 PROCNO 1

F1 - Acquisition parameters
 TD 512
 SFO1 600.1327 MHz
 FIDRES 10.523297 Hz
 SW 8.978 ppm
 FnmODE States-TPPI

F2 - Processing parameters
 SI 2048
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 States-TPPI
 SF 600.1300273 MHz
 WDW TRAP
 SSB 2
 LB 0 Hz
 GB 0

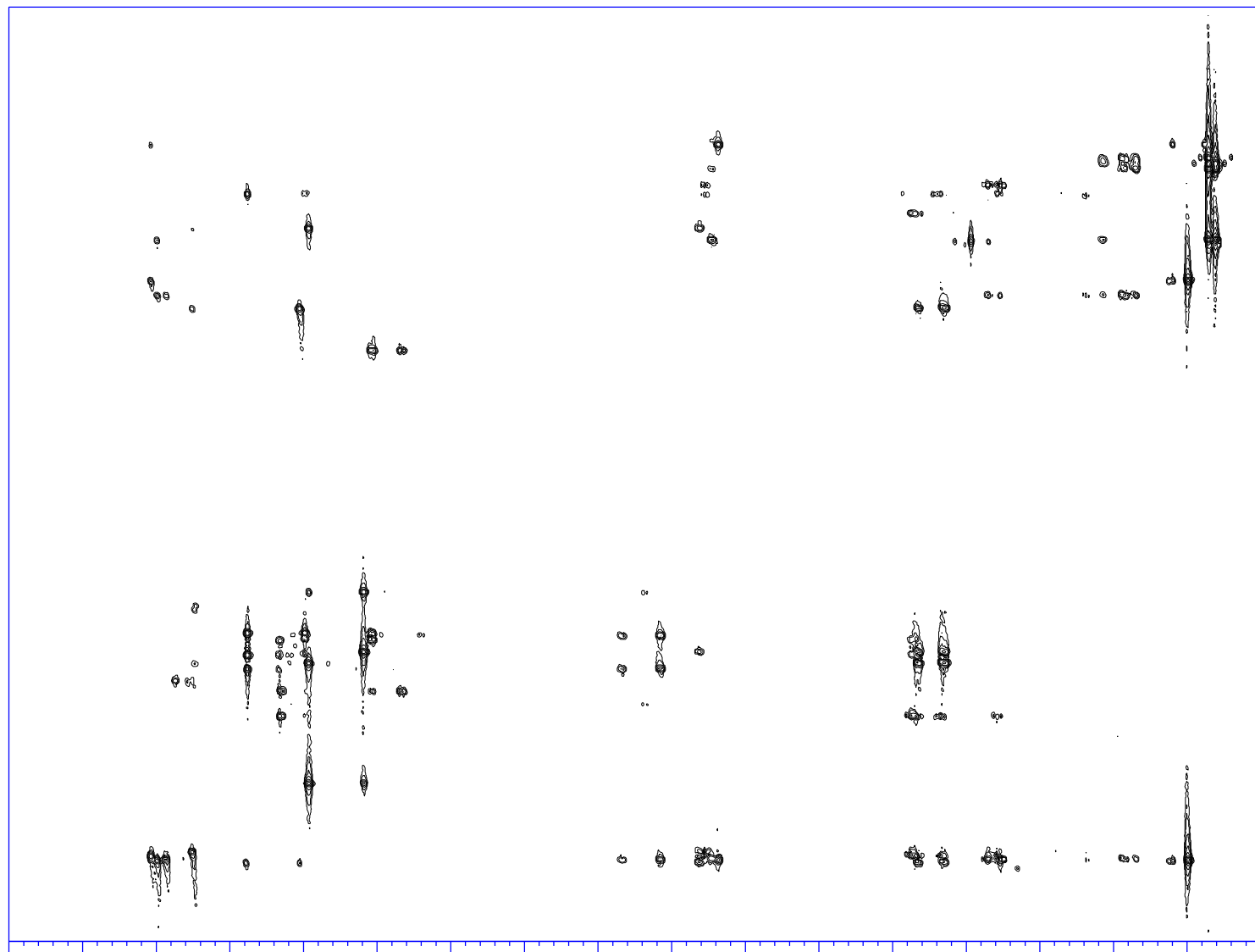
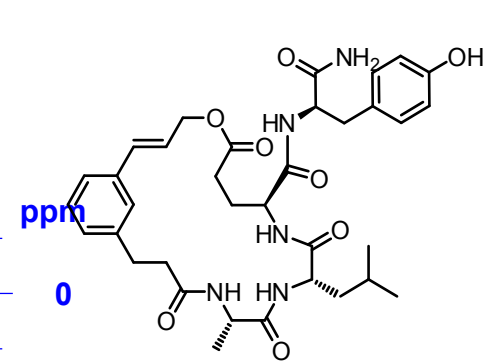
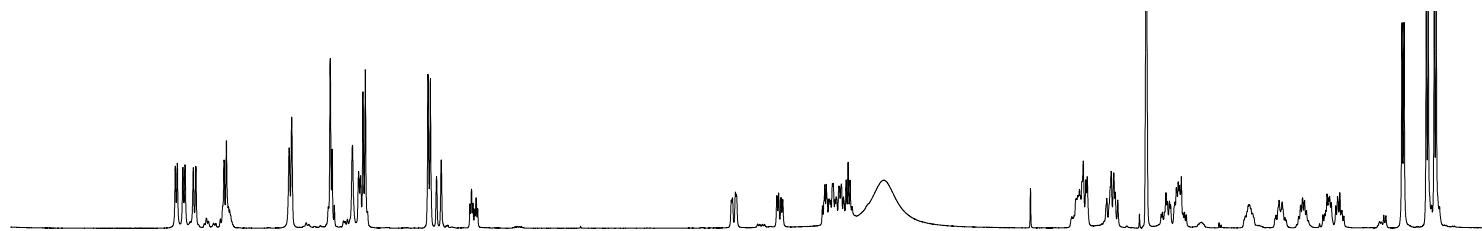


Current Data Parameters
 NAME KL-4-59
 EXPNO 3
 PROCNO 1

F1 - Acquisition parameters
 TD 256
 SFO1 150.9134 MHz
 FIDRES 106.110962 Hz
 SW 180.000 ppm
 FnMODE Echo-Antiecho

F2 - Processing parameters
 SI 2048
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.40

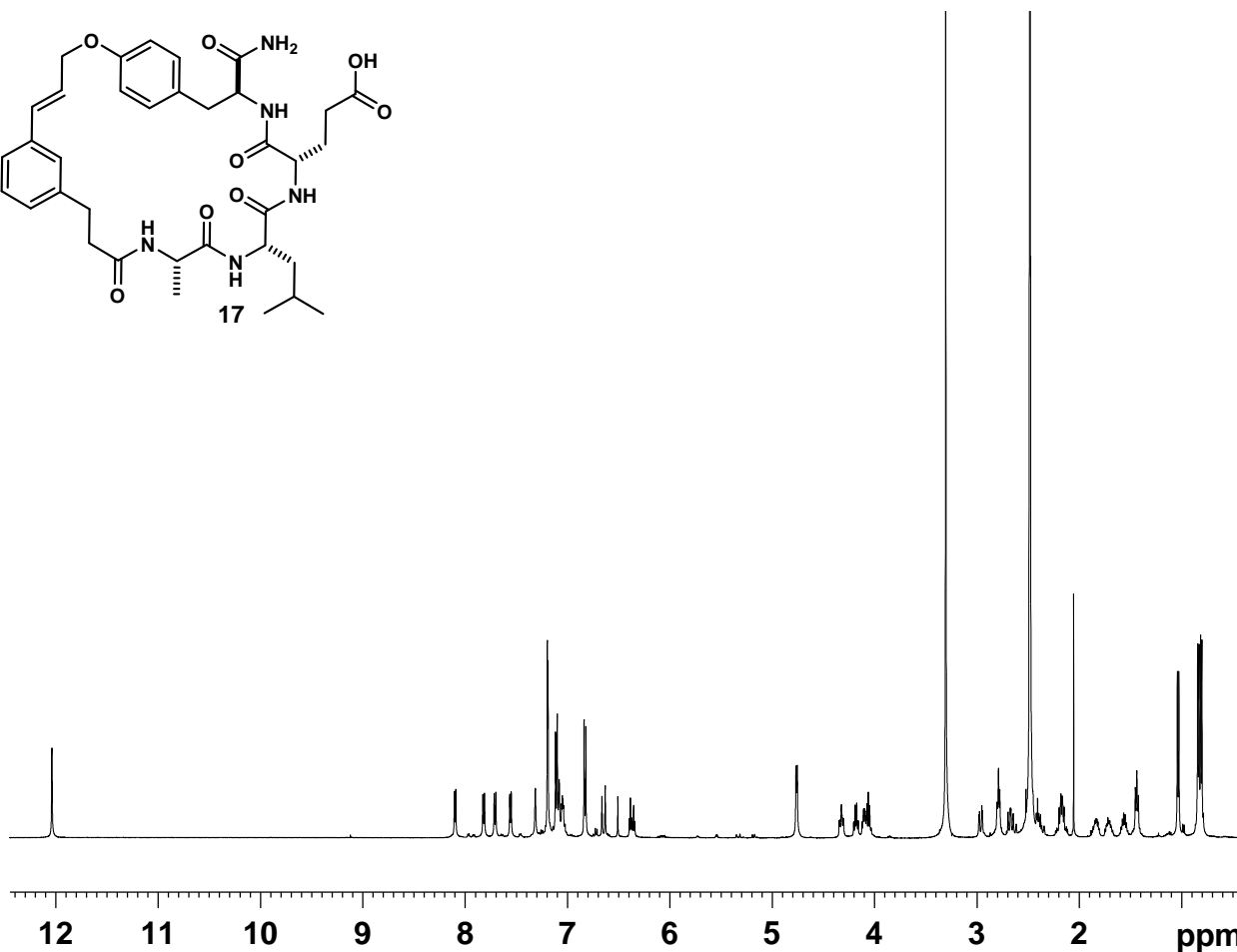
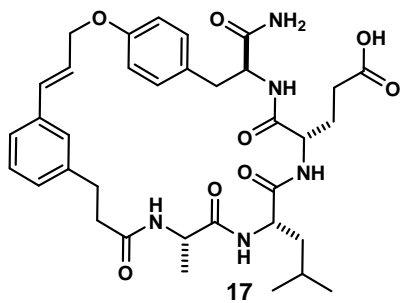
F1 - Processing parameters
 SI 2048
 MC2 echo-antiecho
 SF 150.9028800 MHz
 WDW TRAP
 SSB 2
 LB 0 Hz
 GB 0



Current Data Parameters
 NAME KL-4-59
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111018
 Time 17.34
 INSTRUM av600
 PROBHD 5 mm TBI5
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 16
 DS 16
 SWH 6009.615 Hz
 FIDRES 2.934382 Hz
 AQ 0.1703936 sec
 RG 29193
 DW 83.200 usec
 DE 6.50 usec
 TE 297.4 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 d0 0.00000300 sec
 D1 1.20000005 sec
 d6 0.07142857 sec
 D16 0.00020000 sec
 DELTA1 0.00296667 sec
 DELTA2 0.00192500 sec
 DELTA3 0.07022458 sec
 in0 0 sec
 ST1CNT 256
 d0orig 0.00000300 sec
 phlloop 0
 tlloop 0
 SFO1 600.1330006 MHz
 NUC1 1H
 P1 9.50 usec
 p2 19.00 usec
 PLW1 -1.00000000 W
 SFO2 150.9163903 MHz
 NUC2 13C
 P3 18.50 usec
 PLW2 -1.00000000 W
 GPNAM[1] SINE.100
 GPNAM[2] SINE.100
 GPNAM[3] SINE.100
 GPNAM[4] SINE.100
 GPNAM[5] SINE.100

Cyclic-Ala-Leu-Glu-Tyr (17):

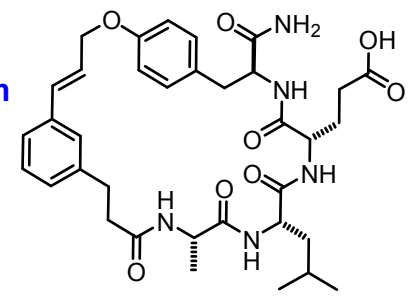
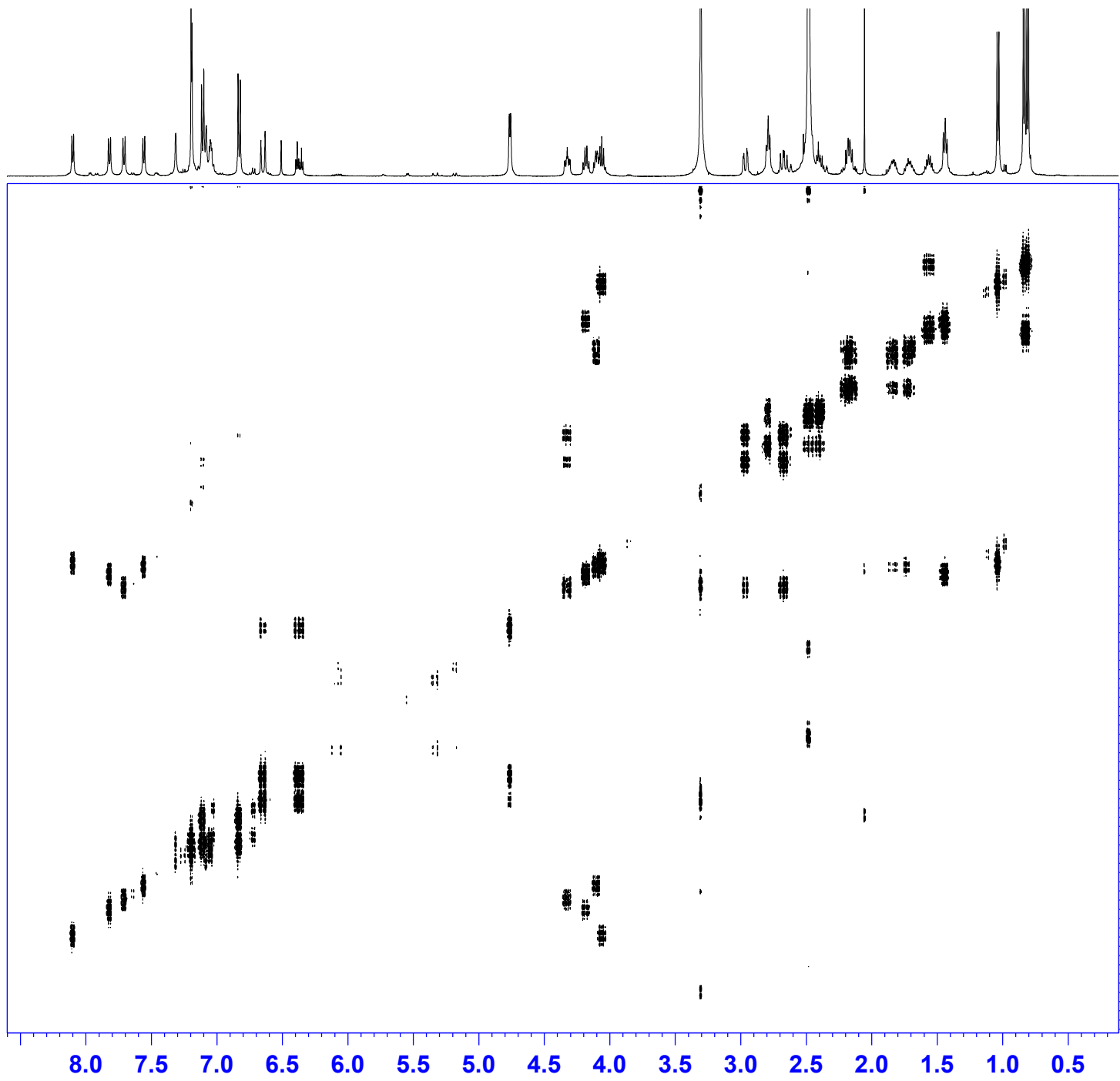


Current Data Parameters
 NAME KL-5-149_F5_AV500
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130326
 Time 17.19
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 14.01
 DW 50.000 usec
 DE 10.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 13.50000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



ppm

0
1
2
3
4
5
6
7
8

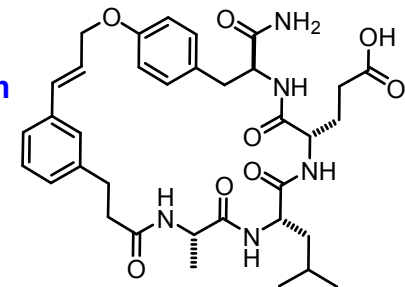
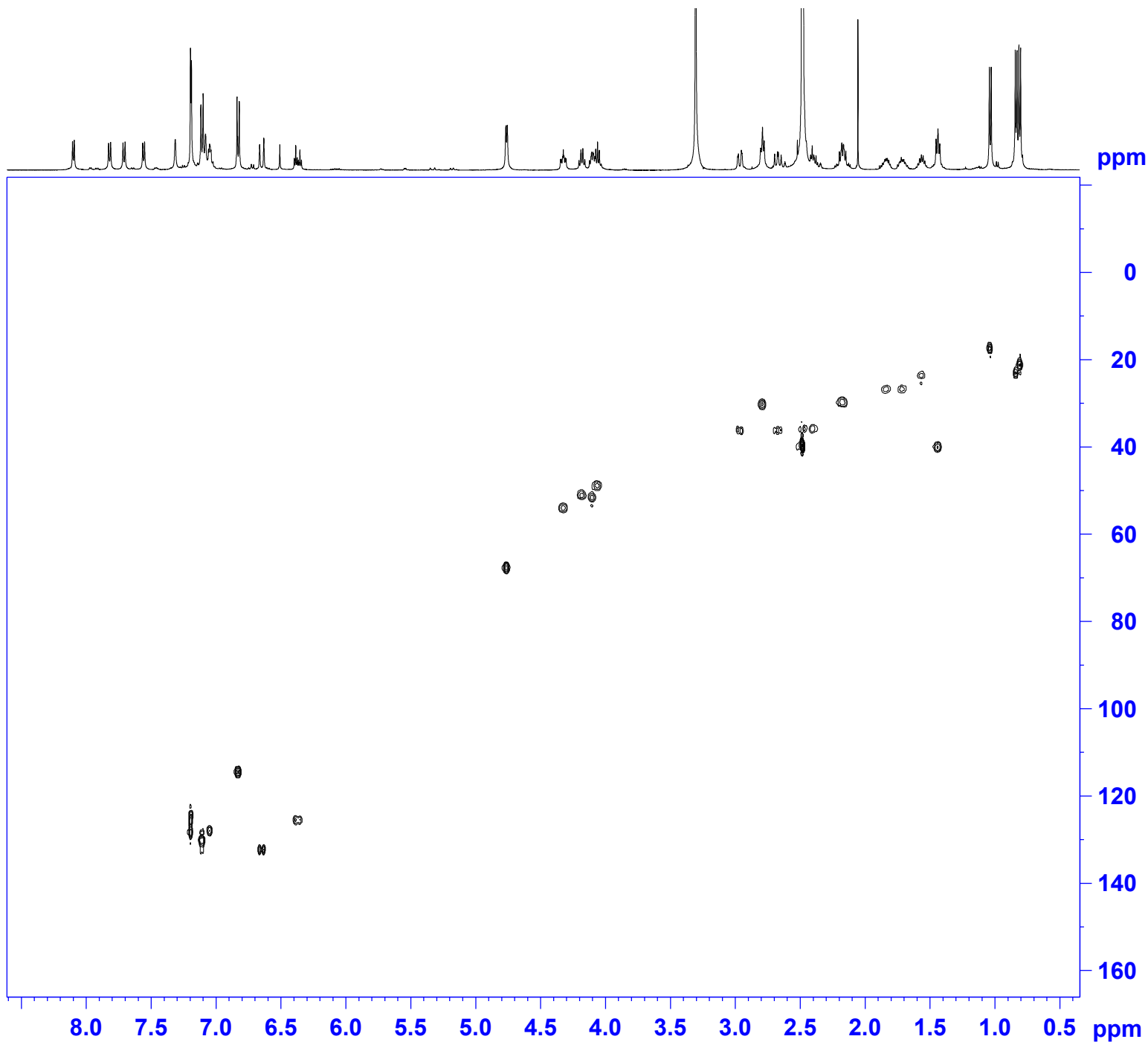
Current Data Parameters
NAME KL-5-149_F5_AV500
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters:
Date_ 20130326
Time 17.21
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG cosygmfph
TD 4096
SOLVENT DMSO
NS 2
DS 8
SWH 5498.534 H:
FIDRES 1.342415 H:
AQ 0.3724629 s:
RG 202.91
DW 90.933 u:
DE 10.00 u:
TE 298.0 K
D0 0.00007880 s:
D1 2.00000000 s:
D13 0.00000400 s:
D16 0.00020000 s:
IN0 0.00018180 s:

===== CHANNEL f1 =====
SFO1 500.1327507 MHz
NUC1 1H
P1 9.50 u:
P2 19.00 u:
PLW1 13.50000000 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 u:

F1 - Acquisition parameters:
TD 256
SFO1 500.1328 MHz
FIDRES 21.486525 H:
SW 10.998 kHz



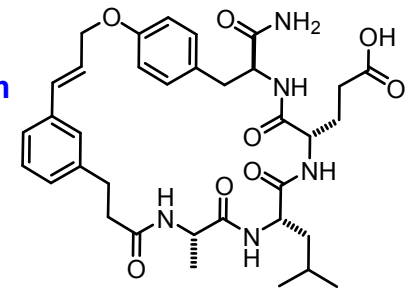
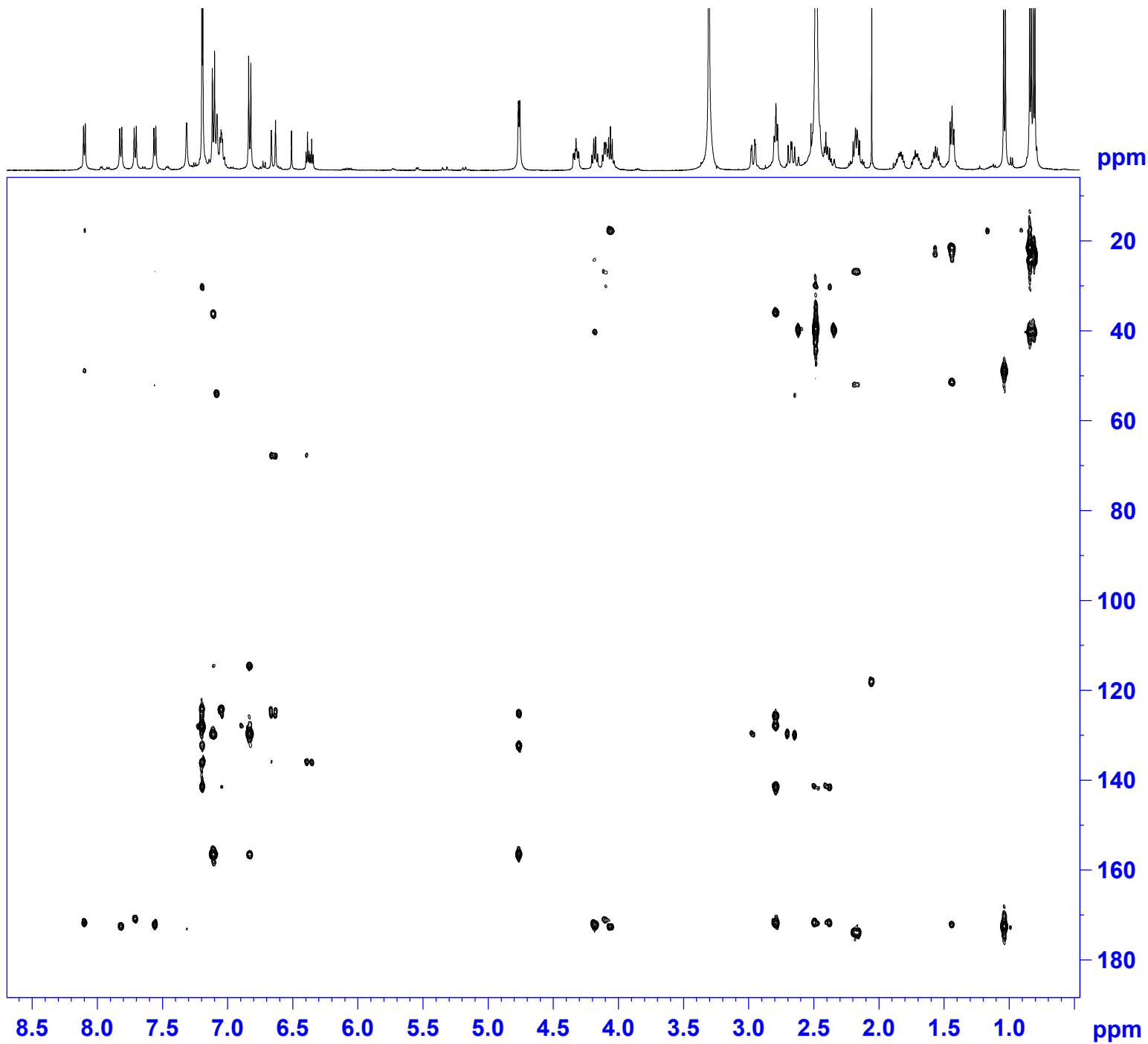
```

Current Data Parameters
NAME      KL-5-149_F5_AV501
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters:
Date_     20130326
Time      17.42
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   hsqcedetgp
TD         2048
SOLVENT   DMSO
NS         2
DS         16
SWH        5000.000 Hz
FIDRES     2.441406 Hz
AQ         0.2048000 sec
RG         202.91
DW         100.000 usec
DE         10.00 usec
TE         298.0 K
CNST2     145.0000000
D0         0.00000300 sec
D1         1.50000000 sec
D4         0.00172414 sec
D11        0.03000000 sec
D13        0.00000400 sec
D16        0.00020000 sec
D21        0.00345000 sec
IN0        0.00001990 sec
ZGOPTNS

===== CHANNEL f1 =====
SFO1       500.1325007 MHz
NUC1       1H
P1         9.50 usec
P2         19.00 usec
P28        0 usec
PLW1       13.50000000 W

===== CHANNEL f2 =====
SFO2       125.7678496 MHz
NUC2       13C
CPDPRG[2]  garp
P3         9.63 usec
P4         19.26 usec
  
```



Current Data Parameters
 NAME KL-5-149_F5_AV501
 EXPNO 5
 PROCNO 1

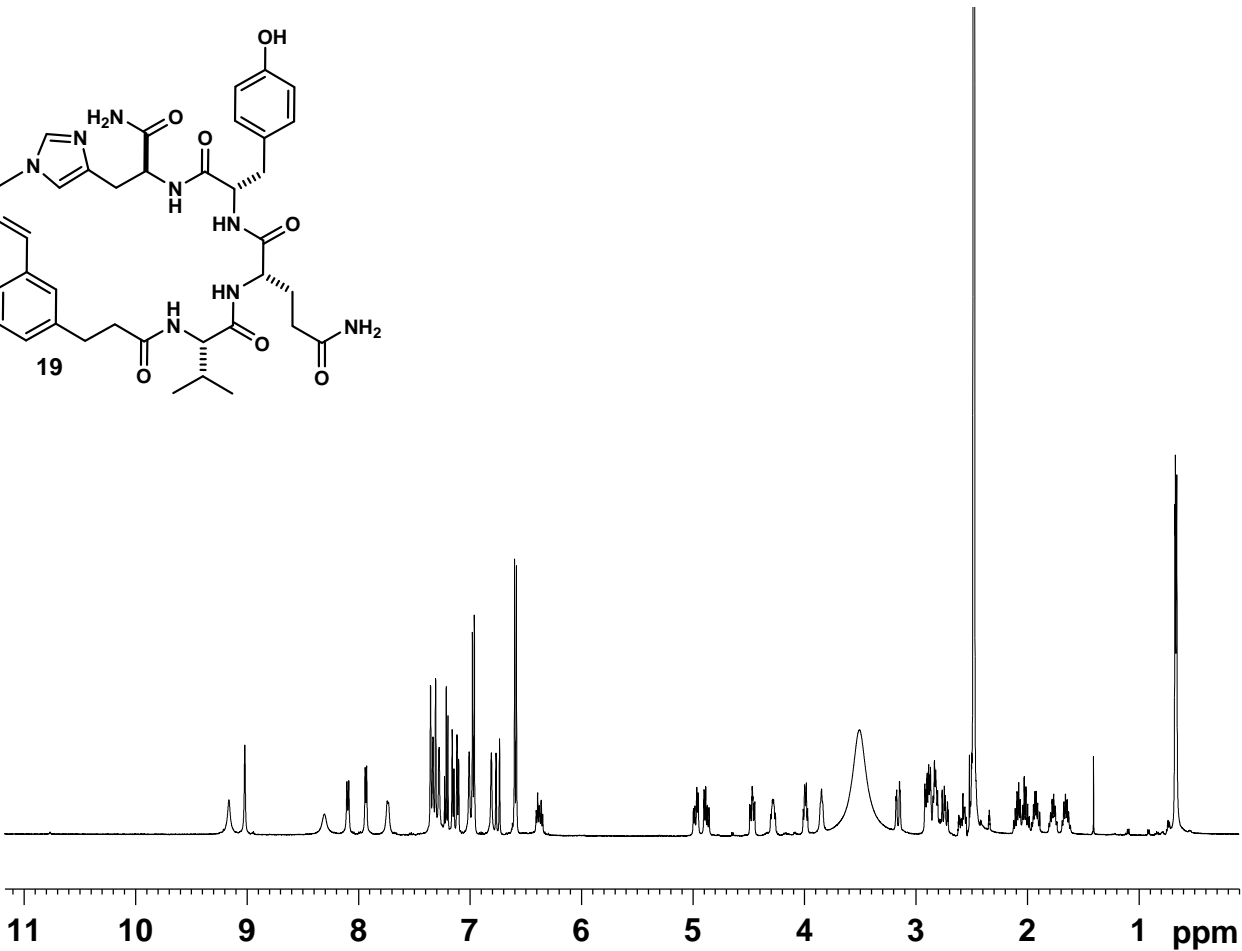
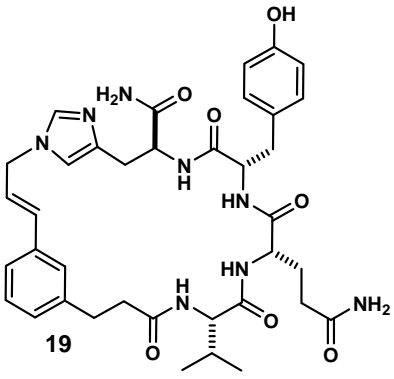
F2 - Acquisition Parameters:
 Date_ 20130326
 Time 17.57
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 202.91
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D6 0.07142857 s:
 D16 0.00020000 s:
 IN0 0.00001990 s:

==== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 PLW1 13.50000000 W

==== CHANNEL f2 =====
 SFO2 125.7703648 MHz
 NUC2 13C
 P3 9.63 u:
 PLW2 23.01399994 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100

Cyclic-Val-Gln-Tyr-His (19):



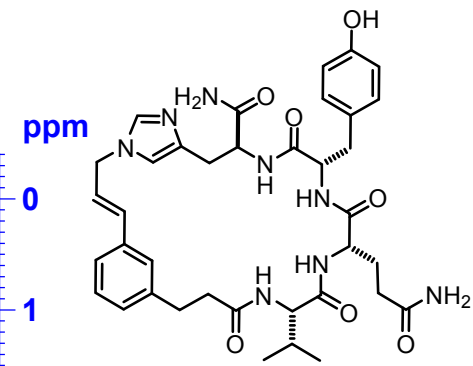
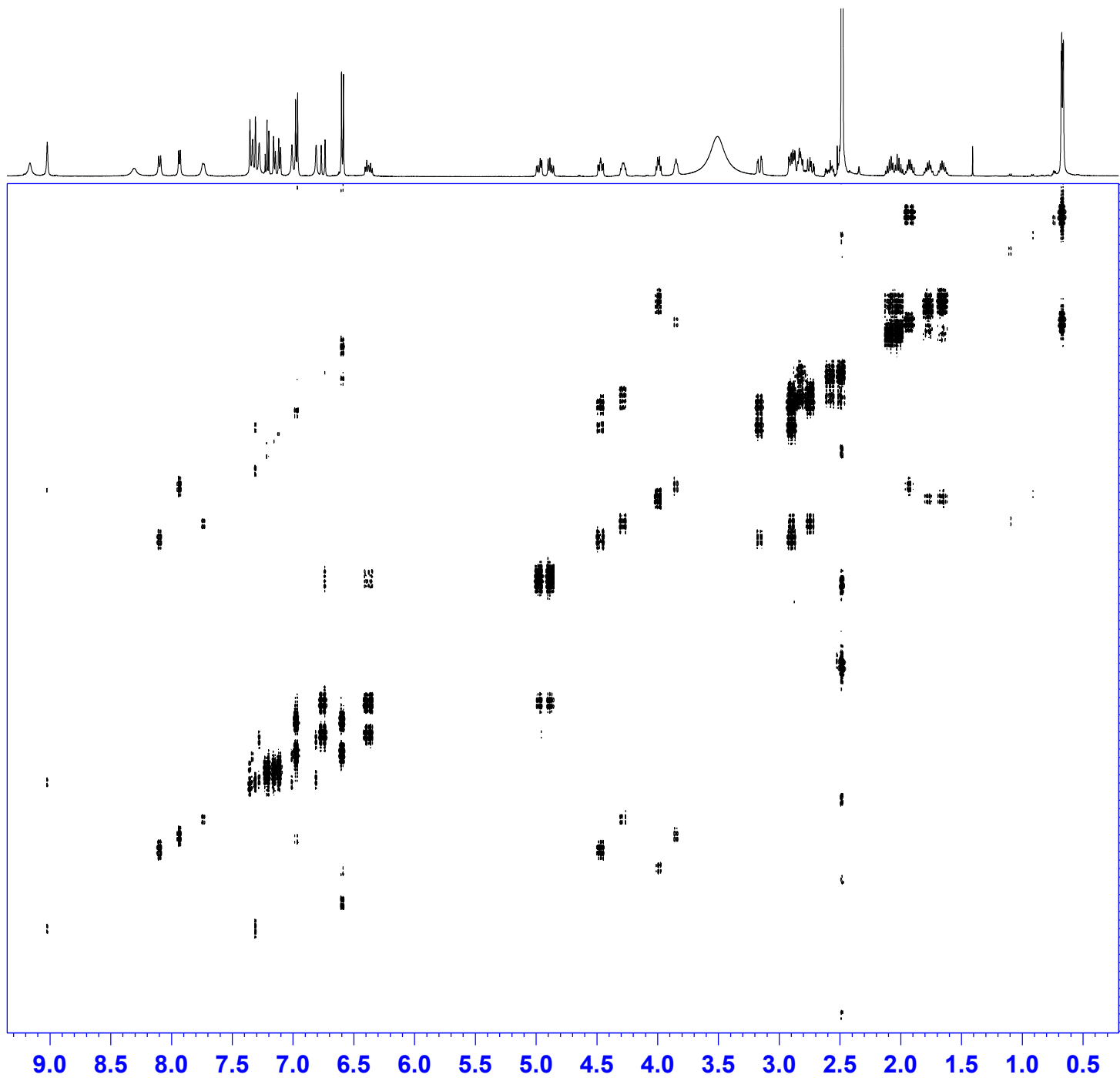
```

Current Data Parameters
NAME      KL-5-152A_F9
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130407
Time     15.08
INSTRUM av500
PROBHD   5 mm DCH 13C-1
PULPROG zg30
TD       65536
SOLVENT  DMSO
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       11
DW       50.000 usec
DE       10.00 usec
TE       298.0 K
D1       2.00000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1    500.1330008 MHz
NUC1     1H
P1       10.00 usec
PLW1    13.50000000 W

F2 - Processing parameters
SI       65536
SF       500.1300146 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



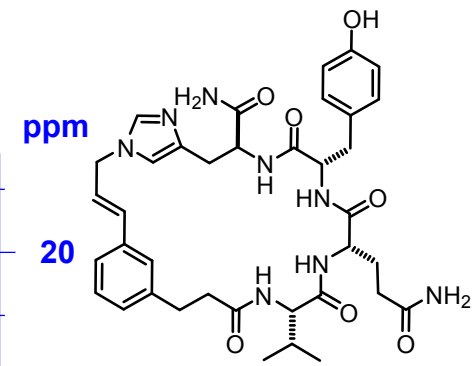
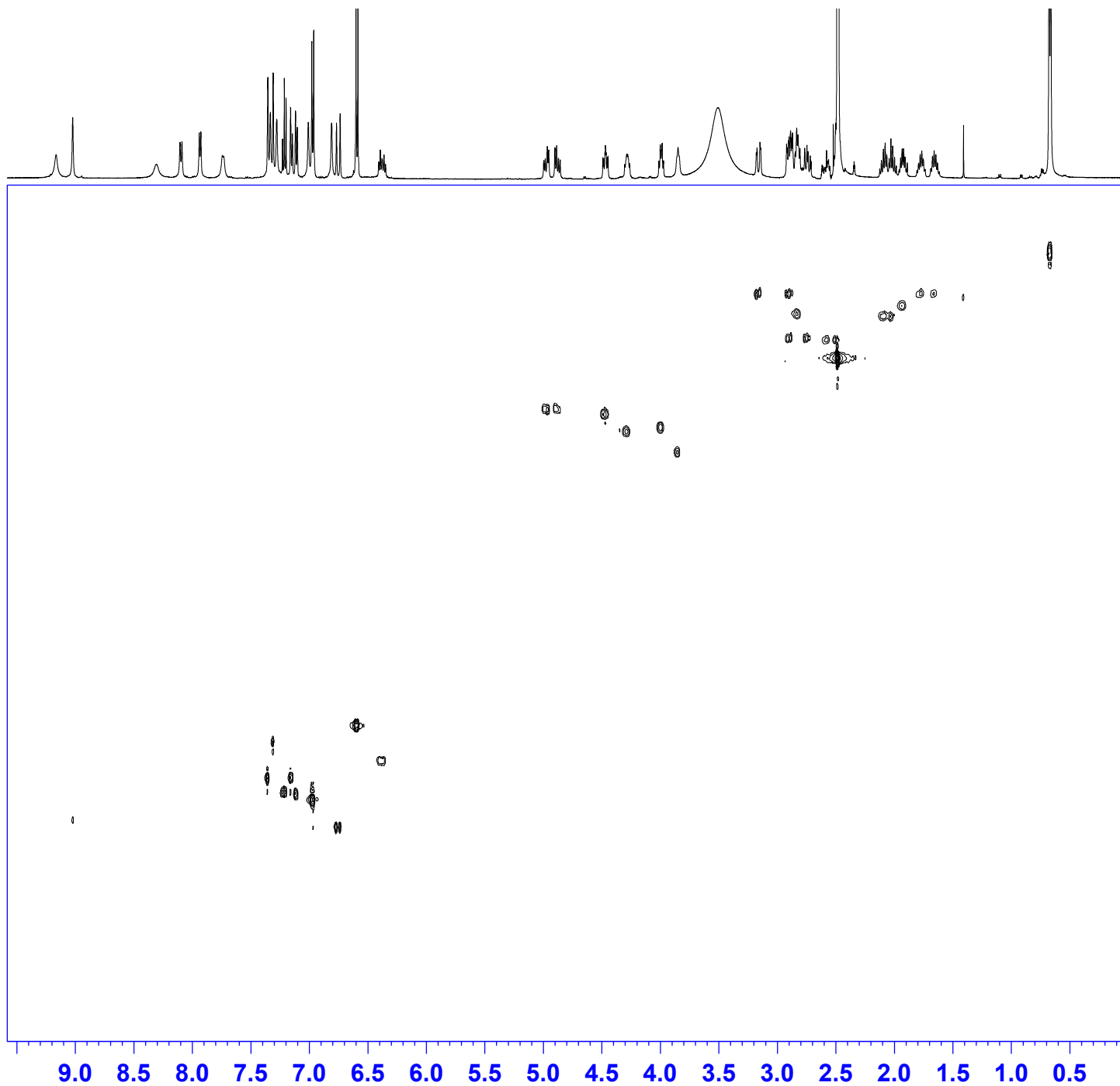
Current Data Parameters
 NAME KL-5-152A_F9
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20130407
 Time 15.11
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG cosygmfph
 TD 4096
 SOLVENT DMSO
 NS 2
 DS 8
 SWH 5498.534 H:
 FIDRES 1.342415 H:
 AQ 0.3724629 s:
 RG 202.91
 DW 90.933 u:
 DE 10.00 u:
 TE 298.0 K
 D0 0.00007880 s:
 D1 2.00000000 s:
 D13 0.00000400 s:
 D16 0.00020000 s:
 IN0 0.00018180 s:

==== CHANNEL f1 =====
 SFO1 500.1327507 M:
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 PLW1 13.50000000 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPZ1 10.00 %
 GPZ2 20.00 %
 P16 1000.00 u:

F1 - Acquisition parameters:
 TD 256
 SFO1 500.1328 M:
 FIDRES 21.486525 H:
 SW 10.998 p:

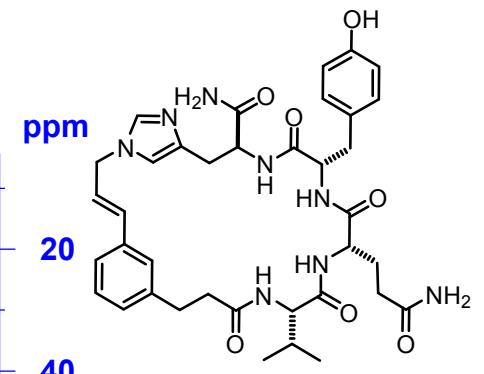
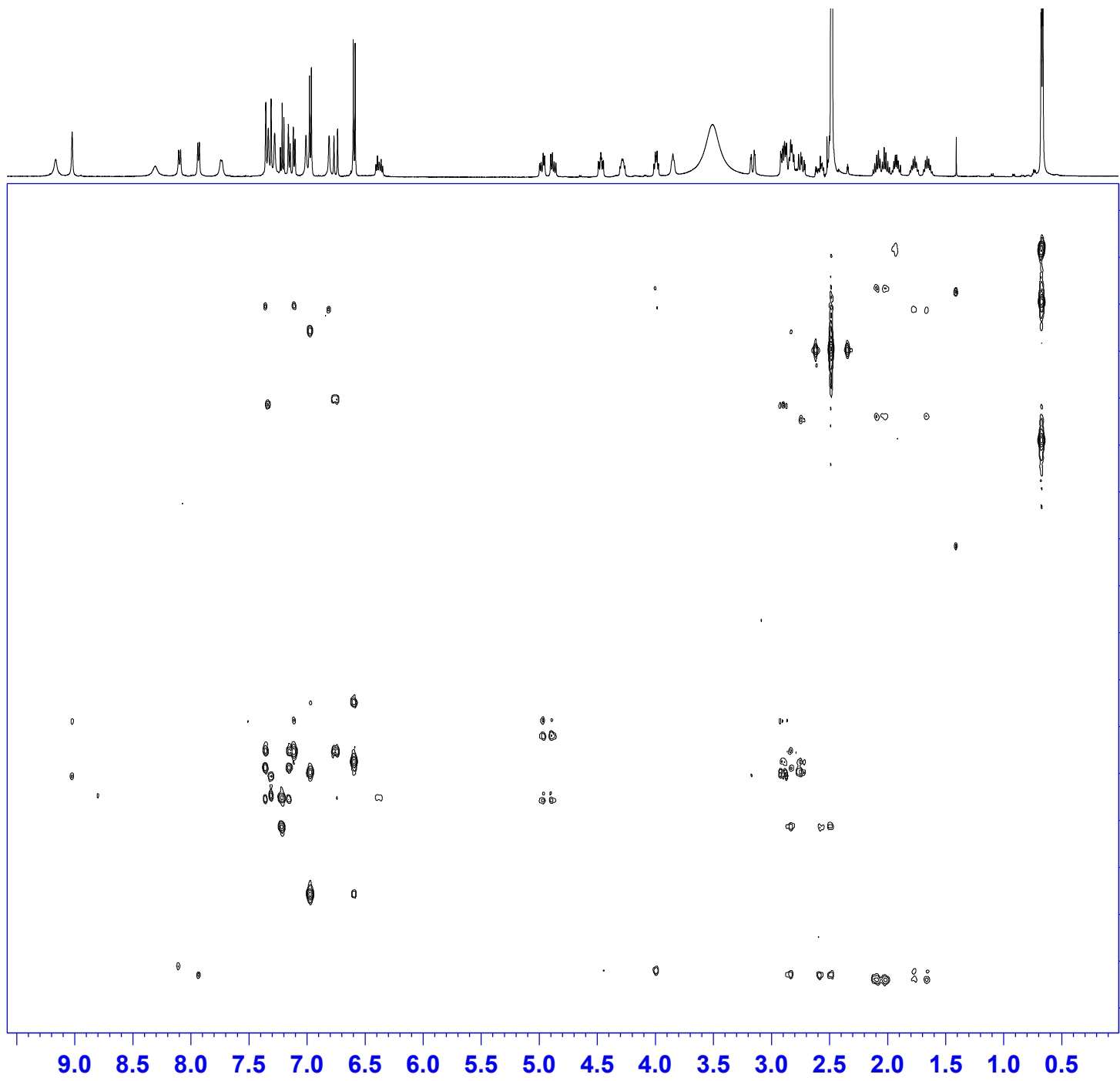


Current Data Parameters
 NAME KL-5-152A_F9
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20130407
 Time 15.32
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hsqcedetgp
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 5000.000 H:
 FIDRES 2.441406 H:
 AQ 0.2048000 s:
 RG 202.91
 DW 100.000 u:
 DE 10.00 u:
 TE 298.0 K
 CNST2 145.0000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D4 0.00172414 s:
 D11 0.03000000 s:
 D13 0.00000400 s:
 D16 0.00020000 s:
 D21 0.00345000 s:
 IN0 0.00001990 s:
 ZGPTNS

===== CHANNEL f1 =====
 SFO1 500.1325007 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 P28 0 usec
 PLW1 13.50000000 W

===== CHANNEL f2 =====
 SFO2 125.7678496 MHz
 NUC2 13C
 CPDPRG[2] garp
 P3 9.63 u:
 P4 19.26 u:



Current Data Parameters
 NAME KL-5-152A_F9
 EXPNO 5
 PROCNO 1

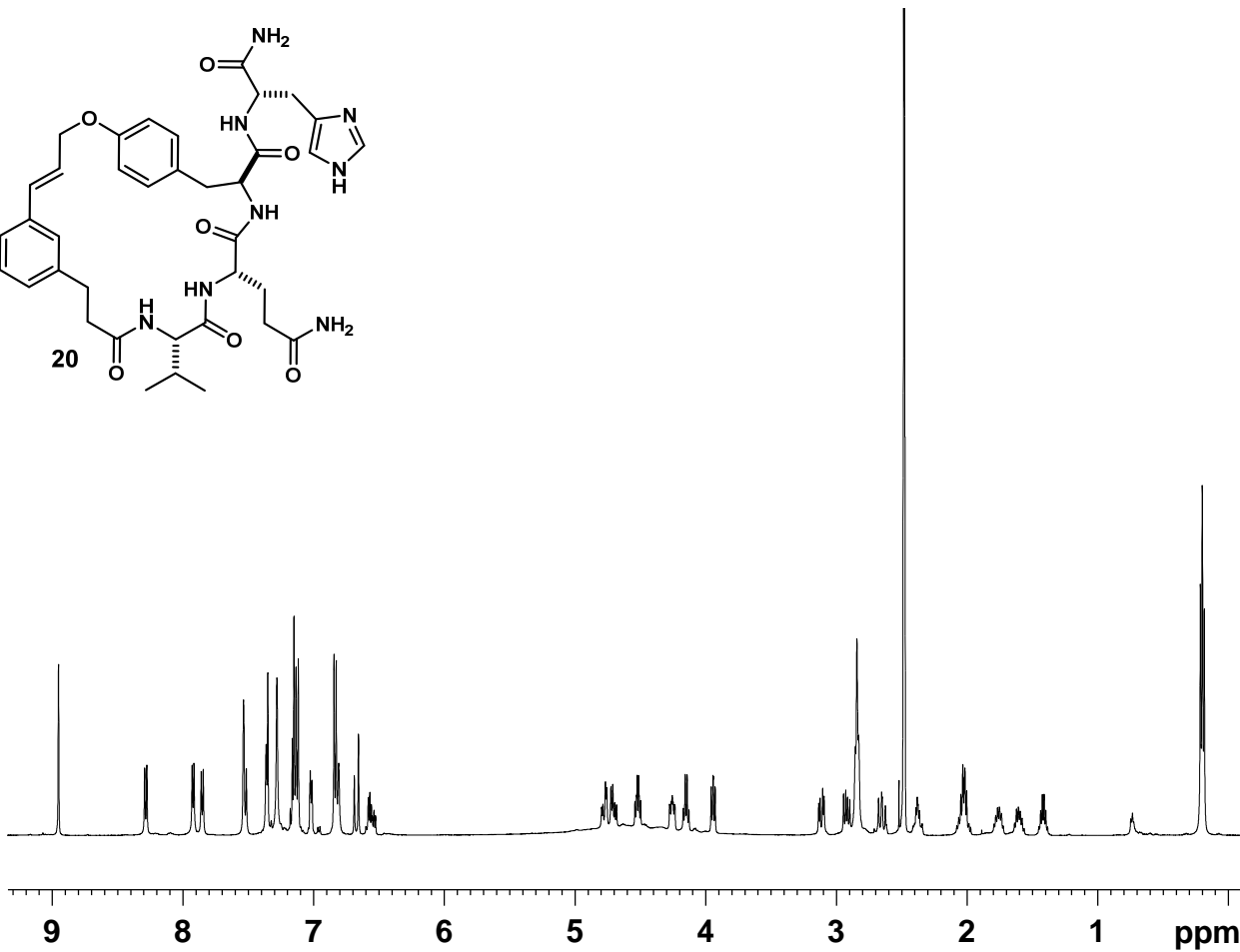
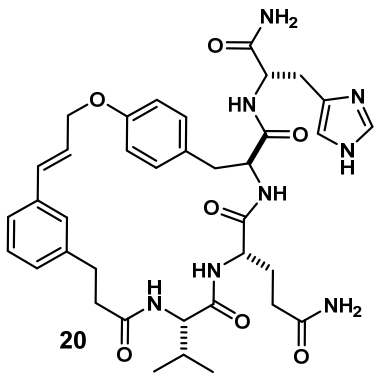
F2 - Acquisition Parameters:
 Date_ 20130407
 Time 15.47
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 202.91
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D6 0.07142857 s:
 D16 0.00020000 s:
 IN0 0.00001990 s:

==== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 PLW1 13.50000000 W

==== CHANNEL f2 =====
 SFO2 125.7703648 MHz
 NUC2 13C
 P3 9.63 u:
 PLW2 23.01399994 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100

Cyclic-Val-Gln-Tyr-His (20):

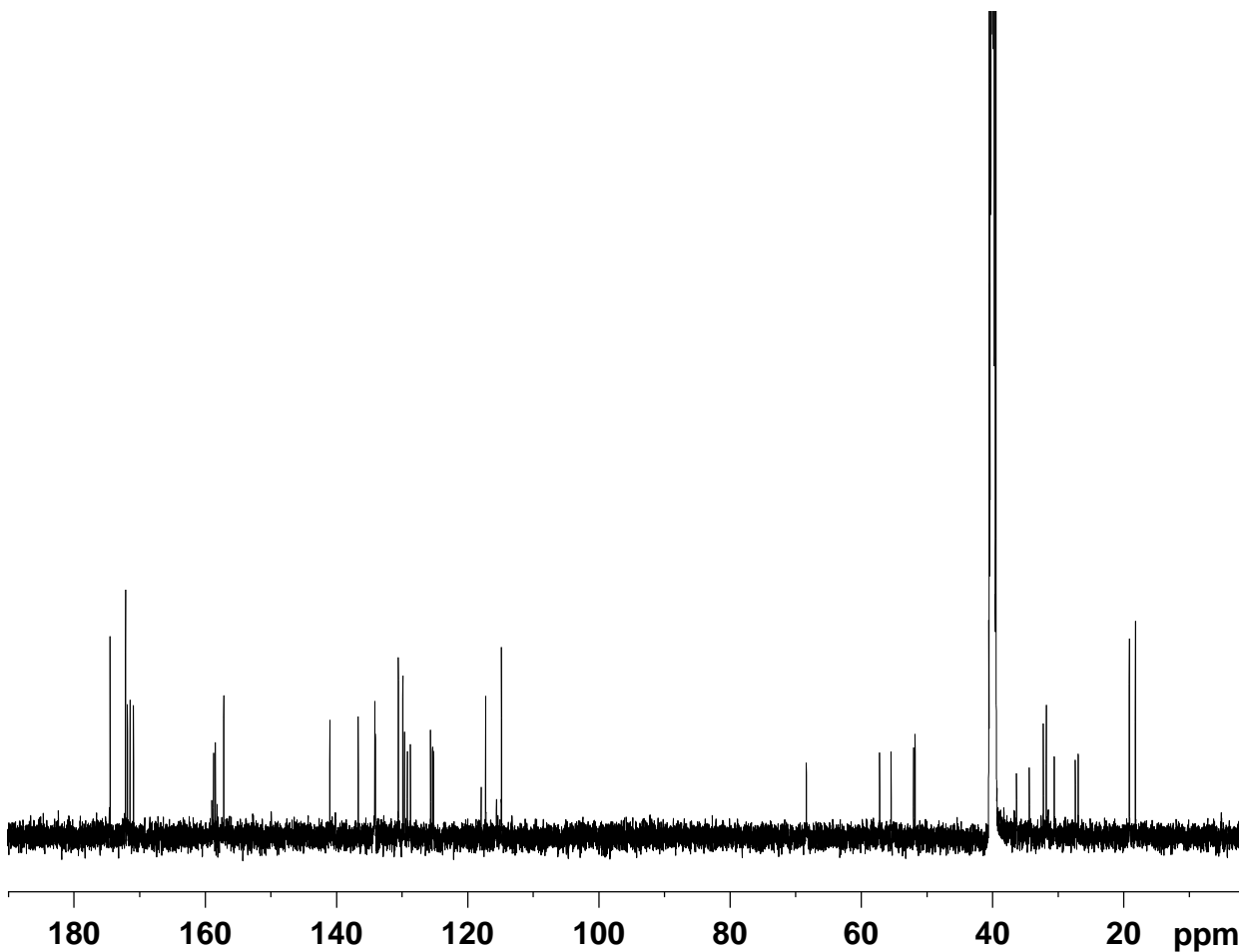


```
Current Data Parameters
NAME      KL-5-159B
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130416
Time     19.50
INSTRUM  av500
PROBHD   5 mm DCH 13C-1
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       28.6
DW       50.000 usec
DE       10.00 usec
TE       298.0 K
D1       2.0000000 sec
D11      1
TD0      1
```

```
===== CHANNEL f1 =====
SFO1    500.1330008 MHz
NUC1    1H
P1      10.00 usec
PLW1    13.5000000 W
```

```
F2 - Processing parameters
SI      65536
SF      500.1300146 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
```



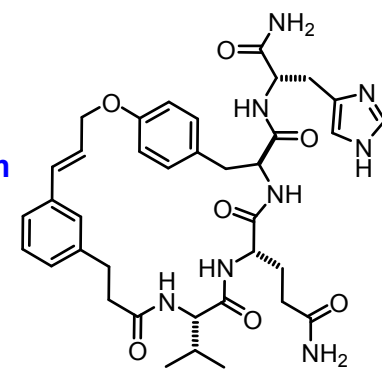
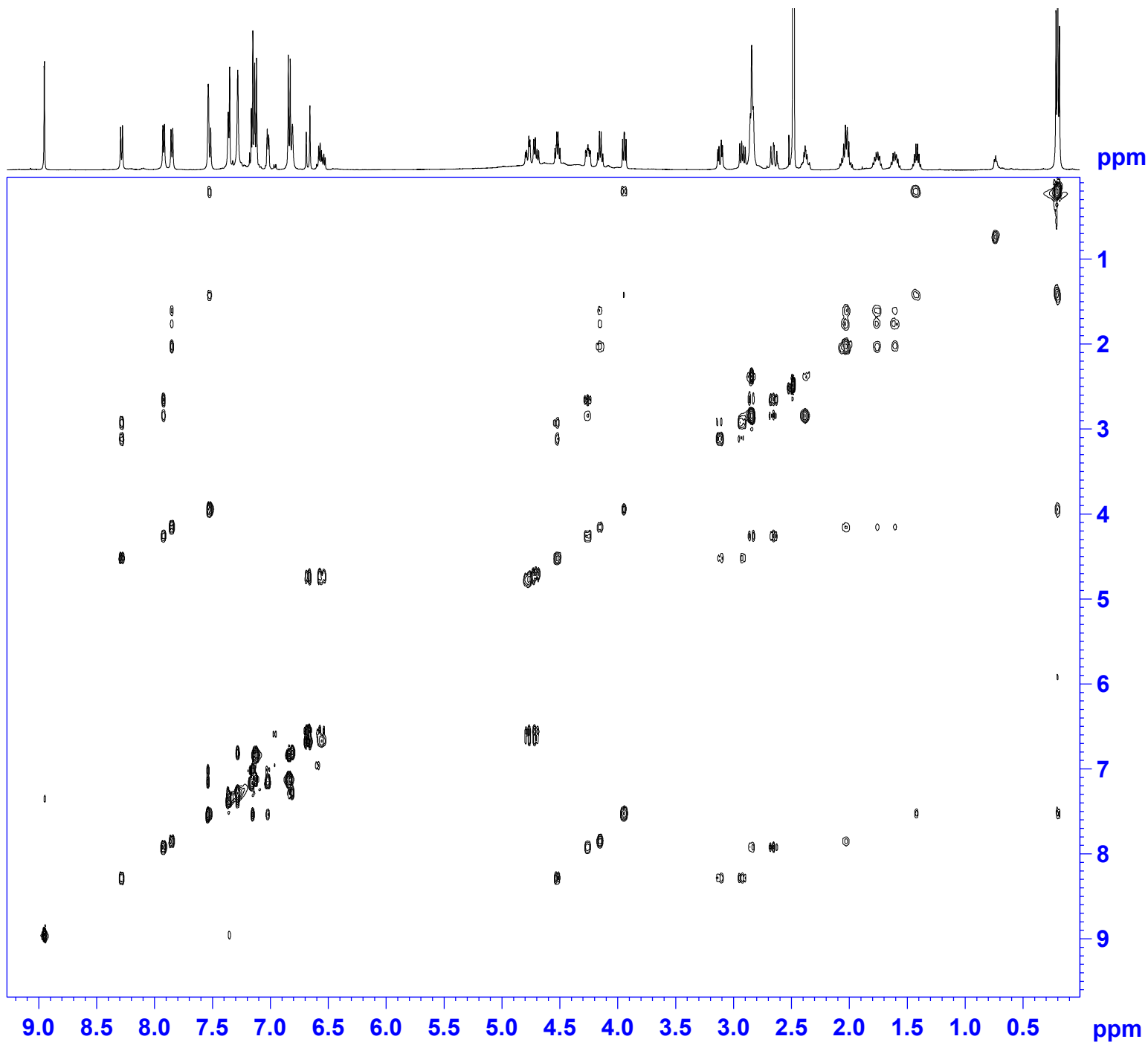
```
Current Data Parameters
NAME      KL-5-159B
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20130416
Time     19.54
INSTRUM  av500
PROBHD   5 mm DCH 13C-1
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       128
DS       2
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0485760 sec
RG       202.91
DW       16.000 usec
DE       18.00 usec
TE       298.0 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
```

```
===== CHANNEL f1 =====
SFO1    125.7722511 MHz
NUC1    13C
P1      9.63 usec
PLW1    23.0000000 W
```

```
===== CHANNEL f2 =====
SFO2    500.1330008 MHz
NUC2    1H
CPDPRG[2] waltz16
PCPD2   80.00 usec
PLW2    13.5000000 W
PLW12   0.21094000 W
PLW13   0.13500001 W
```

```
F2 - Processing parameters
SI      131072
SF      125.7577892 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
```

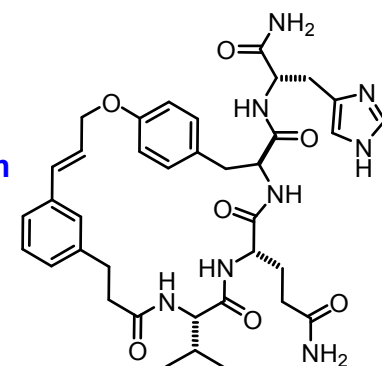
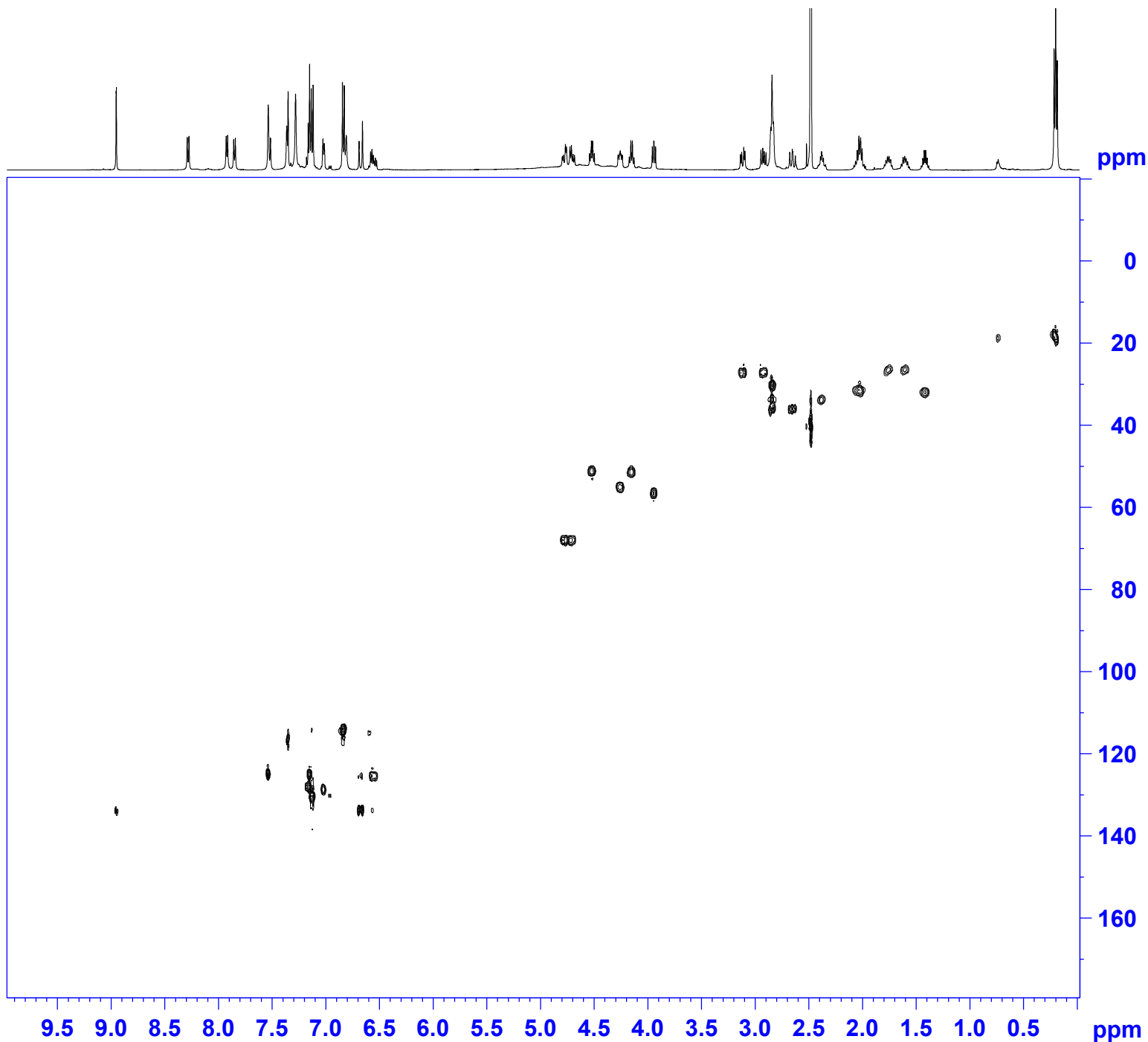


Current Data Parameters
 NAME KL-5-159B
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130417
 Time 19.13
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG mlevetgp.js
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 8
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 37.94
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 D0 0.00000300 s:
 D1 2.00000000 s:
 D9 0.06000000 s:
 D11 0.03000000 s:
 D12 0.00002000 s:
 D16 0.00020000 s:
 IN0 0.00016660 s:
 L1 24

===== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 P5 26.68 u:
 P6 40.00 u:
 P7 80.00 u:
 P17 2500.00 u:
 PLW1 13.5000000 W
 PLW10 0.84375000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SINE.100
 GPNAM[2] SINE.100
 GPZ1 30.00 %

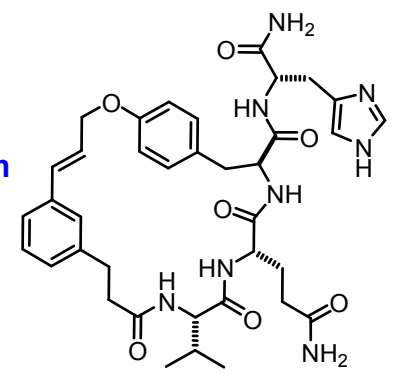
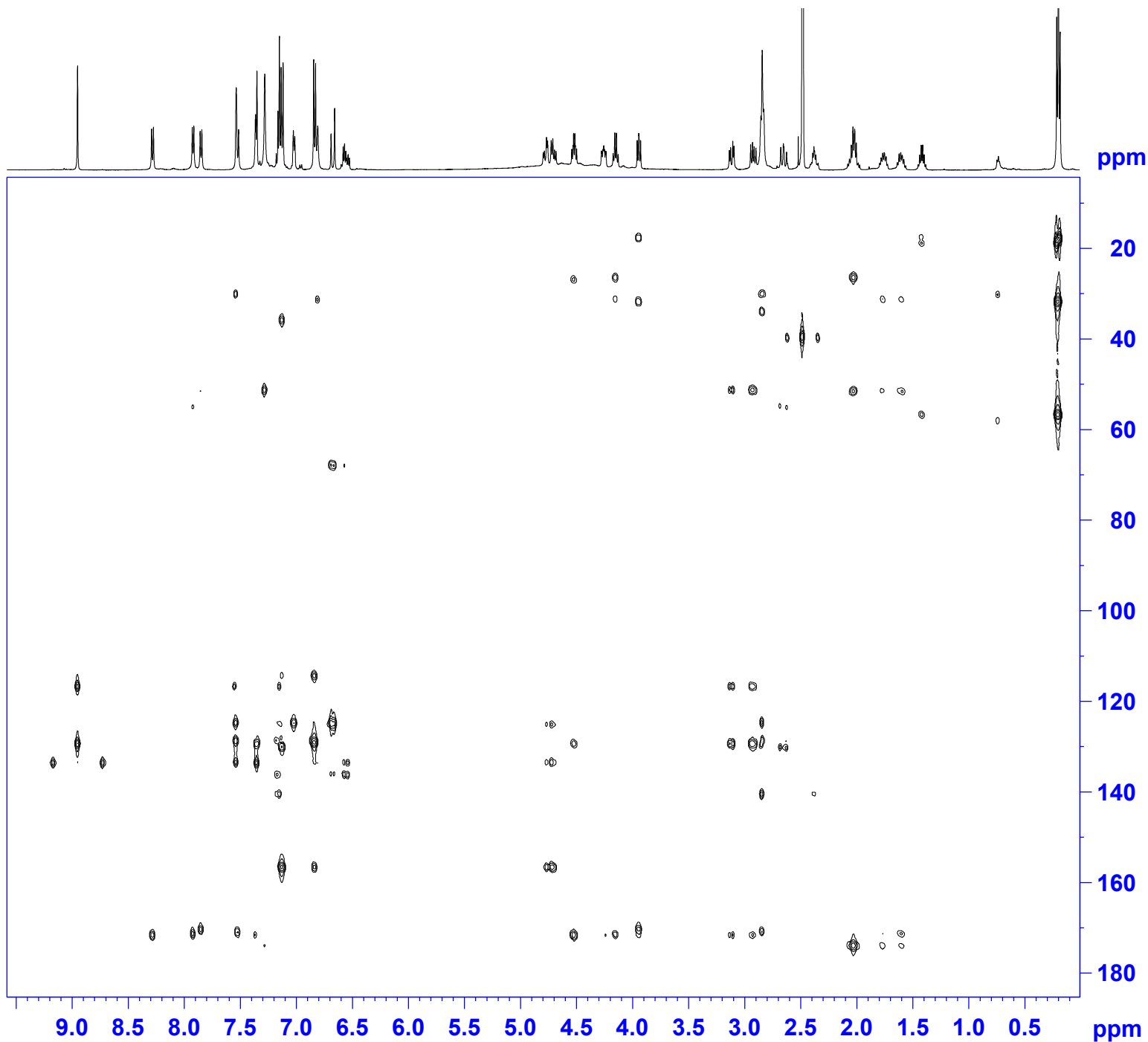


Current Data Parameters
 NAME KL-5-159B
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130417
 Time 19.33
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hsqcedetgp
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 5000.000 H:
 FIDRES 2.441406 H:
 AQ 0.2048000 s:
 RG 202.91
 DW 100.000 u:
 DE 10.00 u:
 TE 298.0 K
 CNST2 145.0000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D4 0.00172414 s:
 D11 0.03000000 s:
 D13 0.00000400 s:
 D16 0.00020000 s:
 D21 0.00345000 s:
 IN0 0.00001990 s:
 ZGOPTNS

==== CHANNEL f1 =====
 SFO1 500.1325007 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 P28 0 usec
 PLW1 13.50000000 W

==== CHANNEL f2 =====
 SFO2 125.7678496 MHz
 NUC2 13C
 CPDPRG[2] garp
 P3 9.63 u:
 P4 19.26 u:



Current Data Parameters
 NAME KL-5-159B
 EXPNO 7
 PROCNO 1

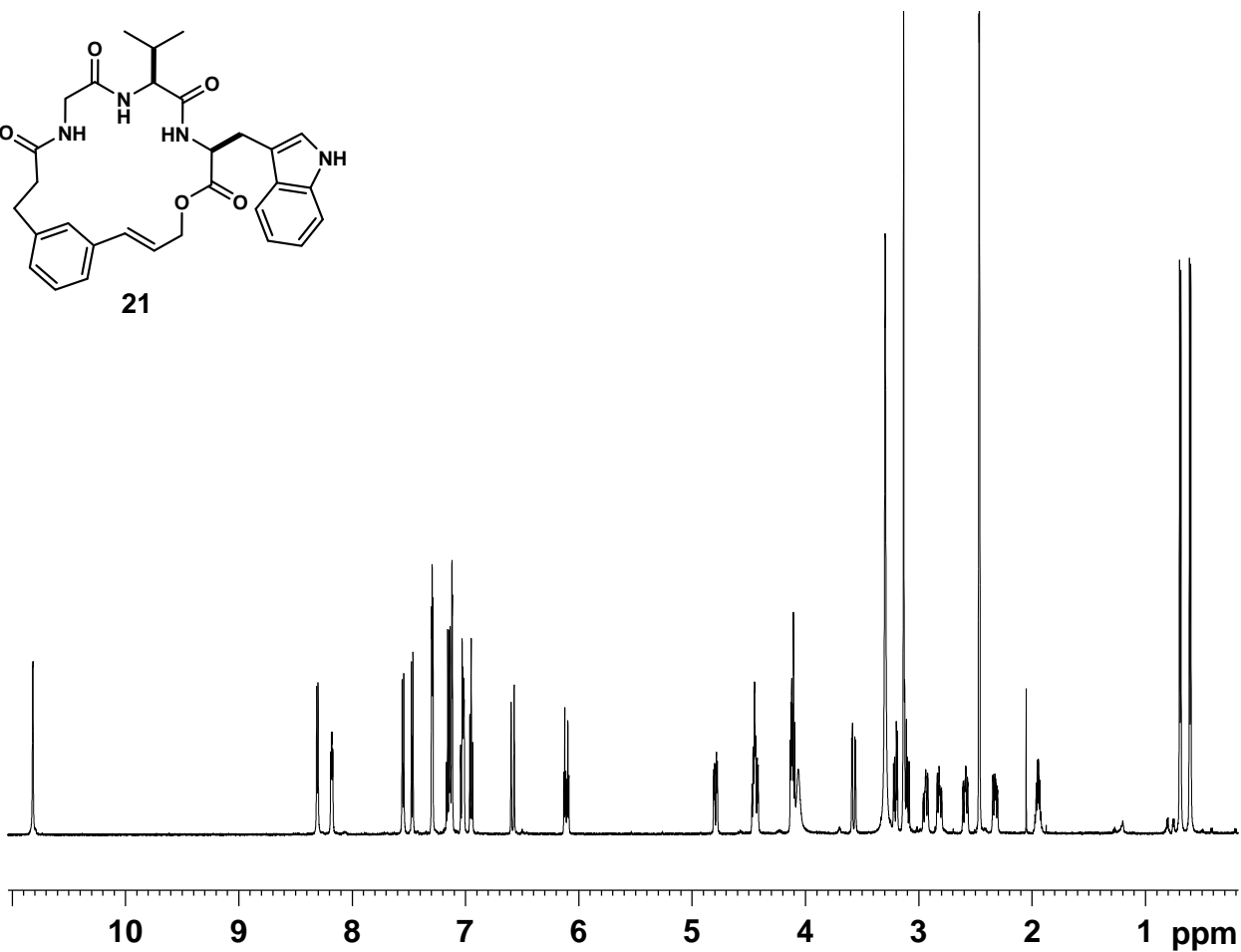
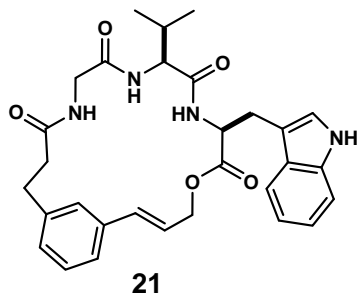
F2 - Acquisition Parameters
 Date_ 20130417
 Time 19.48
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 4
 DS 16
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 202.91
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D6 0.07142857 s:
 D16 0.00020000 s:
 IN0 0.00001990 s:

==== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 PLW1 13.50000000 W

==== CHANNEL f2 =====
 SFO2 125.7703648 MHz
 NUC2 13C
 P3 9.63 u:
 PLW2 23.01399994 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100

Cyclic-Gly-Val-Trp (21):

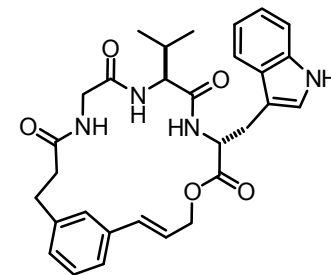
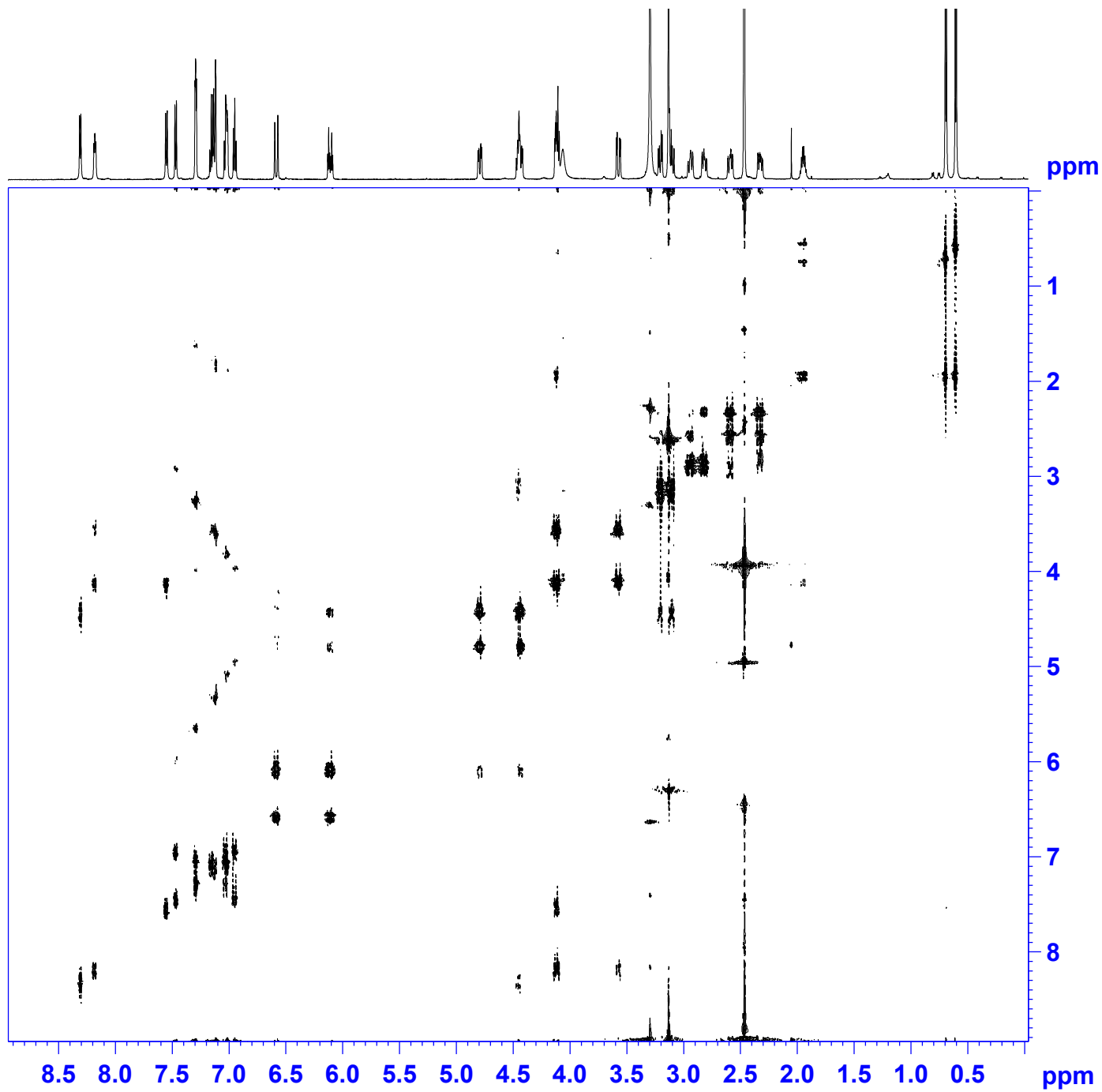


Current Data Parameters
NAME KL-4-189
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120423
Time 11.12
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG zg
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 12376.237 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 181
DW 40.400 usec
DE 6.50 usec
TE 295.7 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -2.00 dB
PL1W 39.81071854 W
SFO1 600.1336008 MHz

F2 - Processing parameters
SI 65536
SF 600.1300273 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

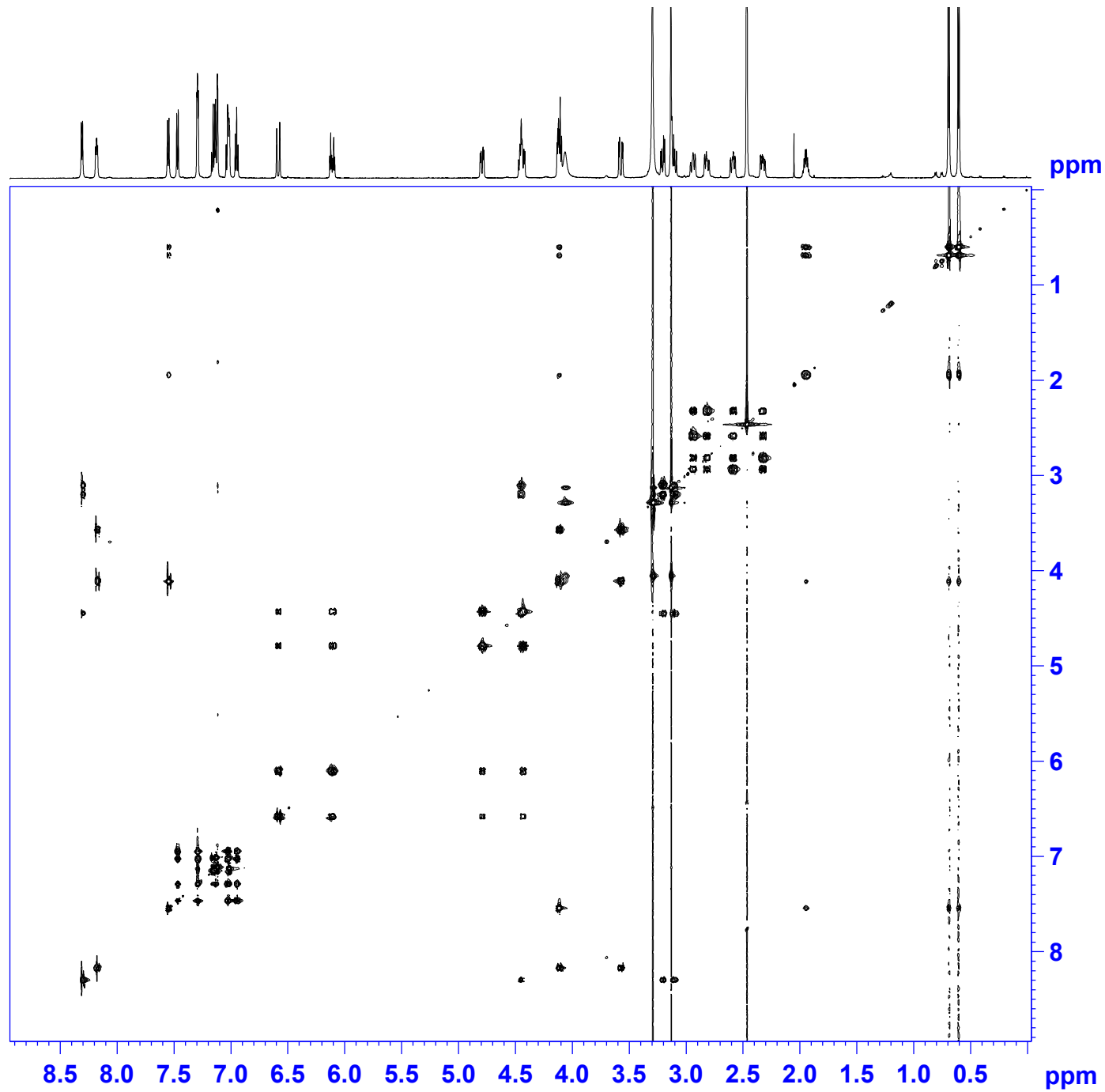
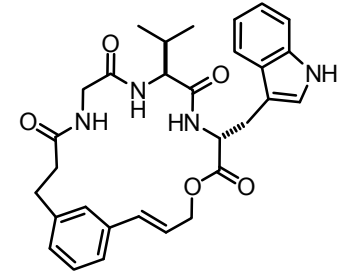


Current Data Parameters

NAME KL-4-189
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20120423
 Time_ 11.15
 INSTRUM av600
 PROBHD 5 mm TBI5
 PULPROG cosygpmfph
 TD 4096
 SOLVENT DMSO
 NS 2
 DS 4
 SWH 5387.931 Hz
 FIDRES 1.315413 Hz
 AQ 0.3801088 sec
 RG 181
 DW 92.800 usec
 DE 6.50 usec
 TE 295.7 K
 d0 -0.00001210 sec
 D1 2.00000000 sec
 d13 0.00000400 sec
 D16 0.00020000 sec
 DELTA 0.00120400 sec
 in0 0 sec
 ST1CNT 256
 d0orig -0.00001210 sec
 phloop 0
 t1loop 0
 SFO1 600.1327006 MHz
 F2 100



Current Data Parameters

NAME KL-4-189
EXPNO 5
PROCNO 1

F1 - Acquisition parameters

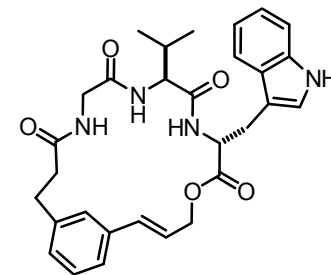
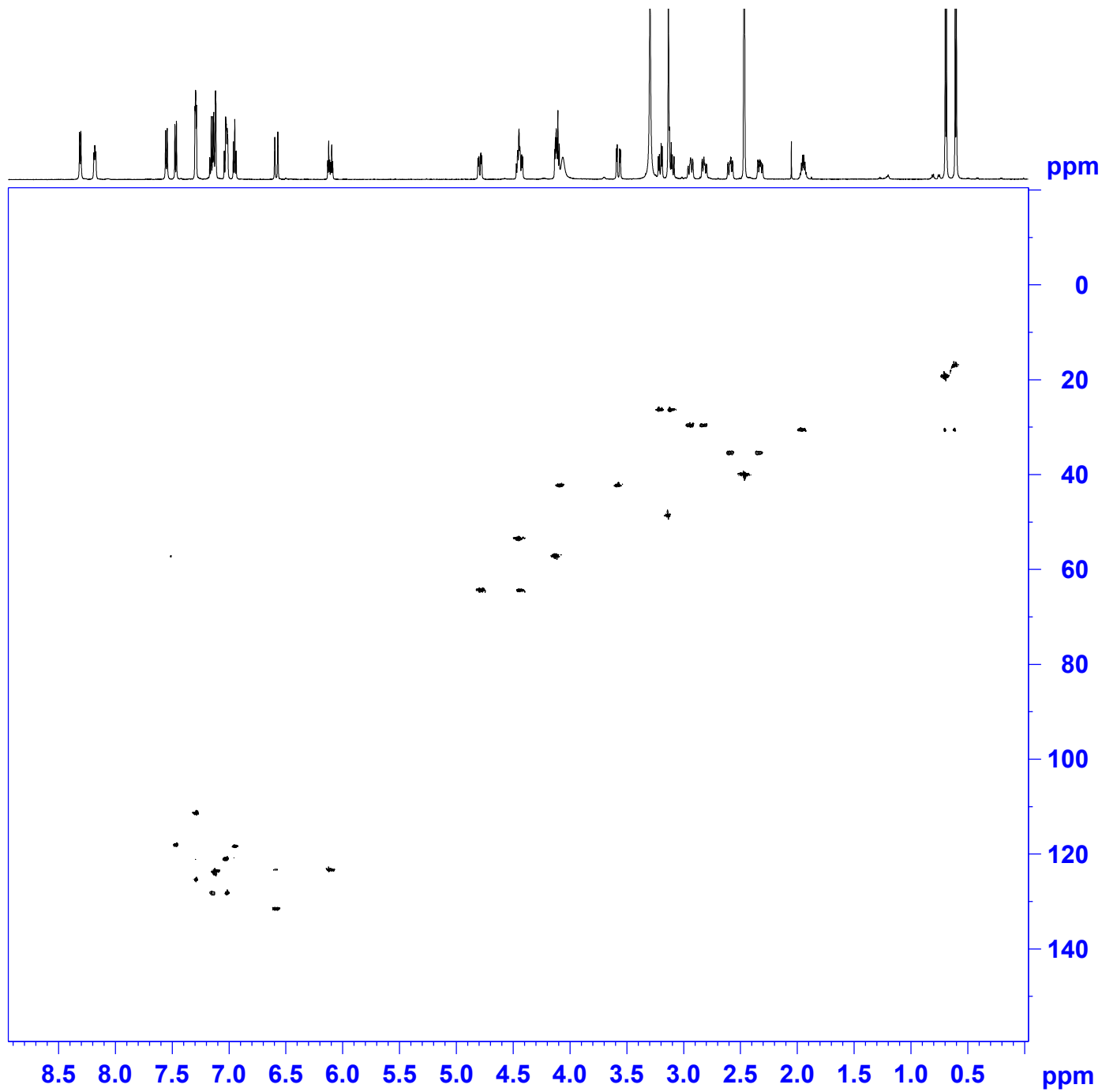
TD 600
SFO1 600.1327 MHz
FIDRES 10.602203 Hz
SW 10.600 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters

SI 1024
SF 600.1300273 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters

SI 1024
MC2 echo-antiecho
SF 600.1300273 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0



0 Current Data Parameters
 NAME KL-4-189
 EXPNO 6
 PROCNO 1

20 F2 - Acquisition Parameters
 Date_ 20120423
 Time_ 12.11

40 INSTRUM av600
 PROBHD 5 mm TBI5
 PULPROG hsqcetgpsisp

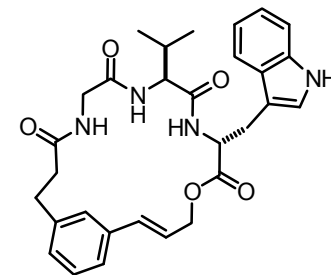
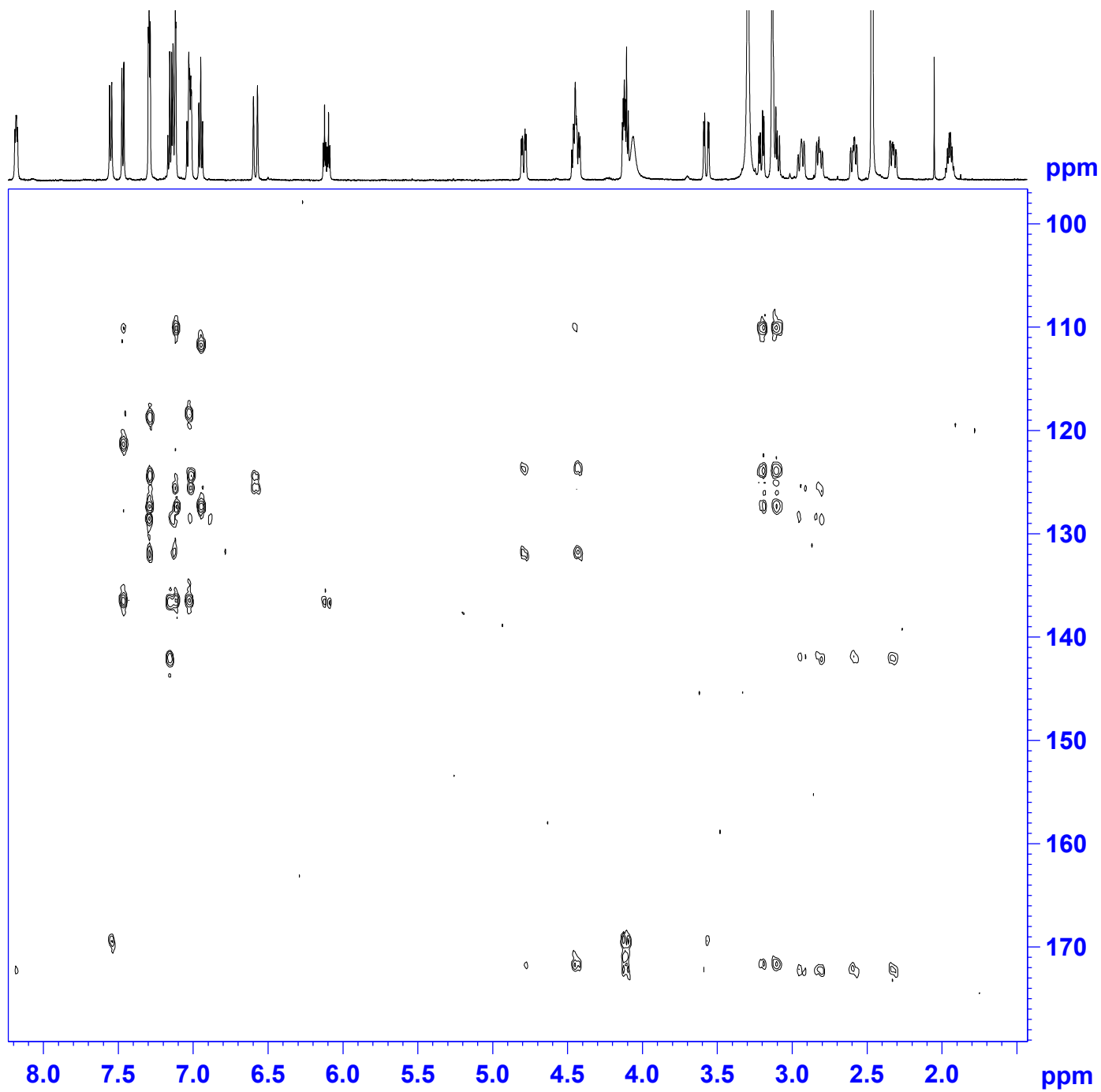
60 TD 2048
 SOLVENT DMSO
 NS 8
 DS 16

80 SWH 5387.931 Hz
 FIDRES 2.630826 Hz
 AQ 0.1900544 sec
 RG 26008

100 DW 92.800 usec
 DE 6.00 usec
 TE 295.8 K

120 CNST2 145.0000000
 d0 0.00000300 sec
 D1 1.20000005 sec
 d4 0.00172414 sec
 d11 0.03000000 sec

140 D16 0.00020000 sec
 D24 0.00086200 sec
 DELTA 0.00127500 sec
 DELTA1 0.00120659 sec
 DELTA2 0.00097414 sec
 in0 0 sec



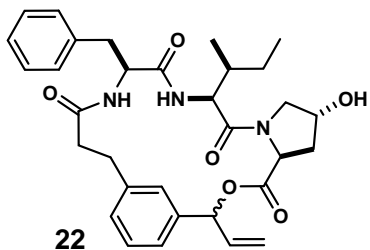
Current Data Parameters

NAME KL-4-189
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20120423
 Time_ 12.59
 INSTRUM av600
 PROBHD 5 mm TBI5
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 8
 DS 16
 SWH 6613.757 Hz
 FIDRES 3.229373 Hz
 AQ 0.1548288 sec
 RG 29193
 DW 75.600 usec
 DE 6.50 usec
 TE 297.8 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 d0 0.00000300 sec
 D1 1.20000005 sec
 d6 0.07142857 sec
 D16 0.00020000 sec
 DELTA1 0.00296667 sec
 DELTA2 0.00192500 sec
 DELTA3 0.07022458 sec
 in0 0 sec

Cyclic-Phe-Leu-Hyp (22):

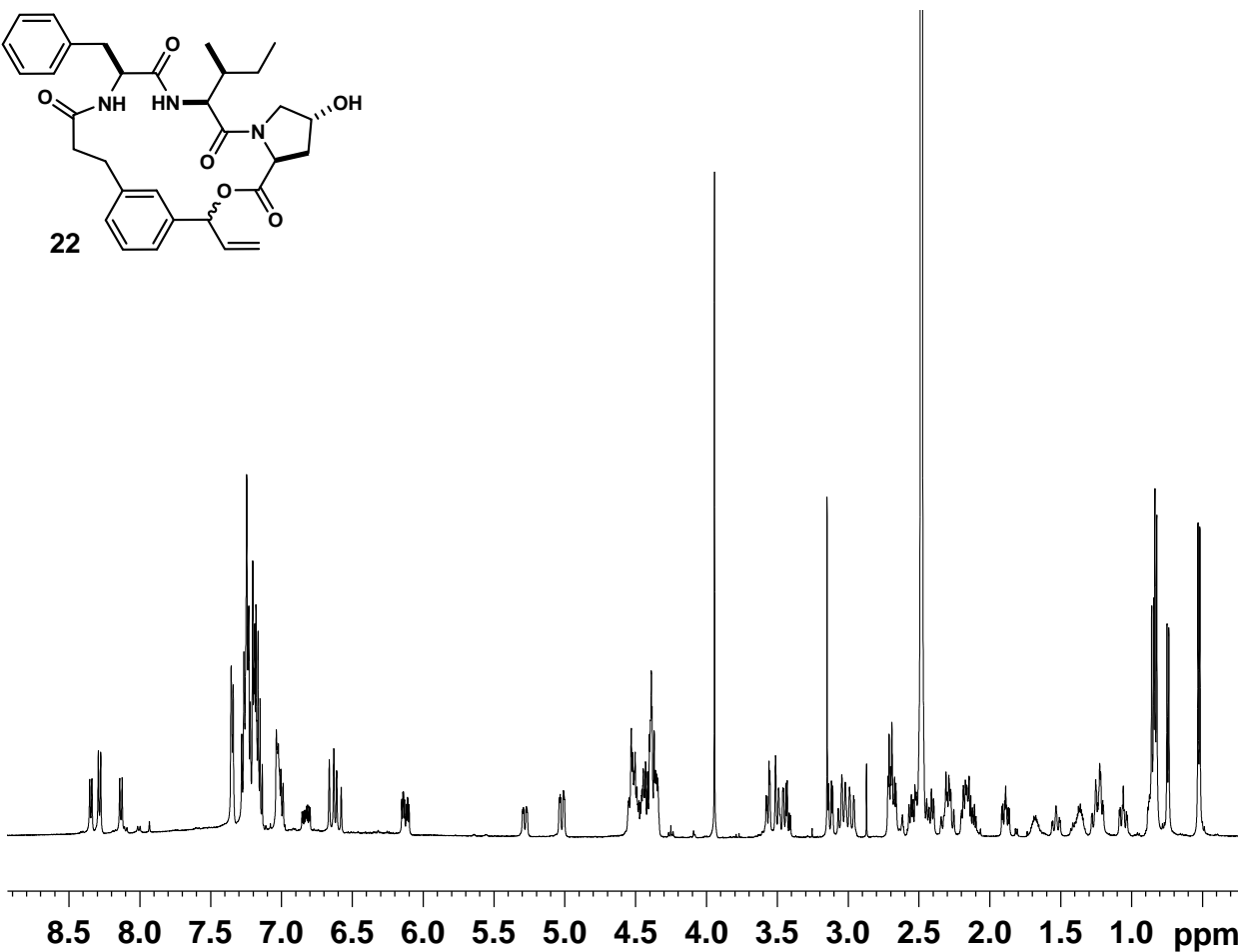


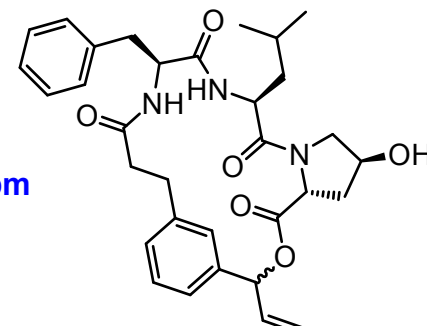
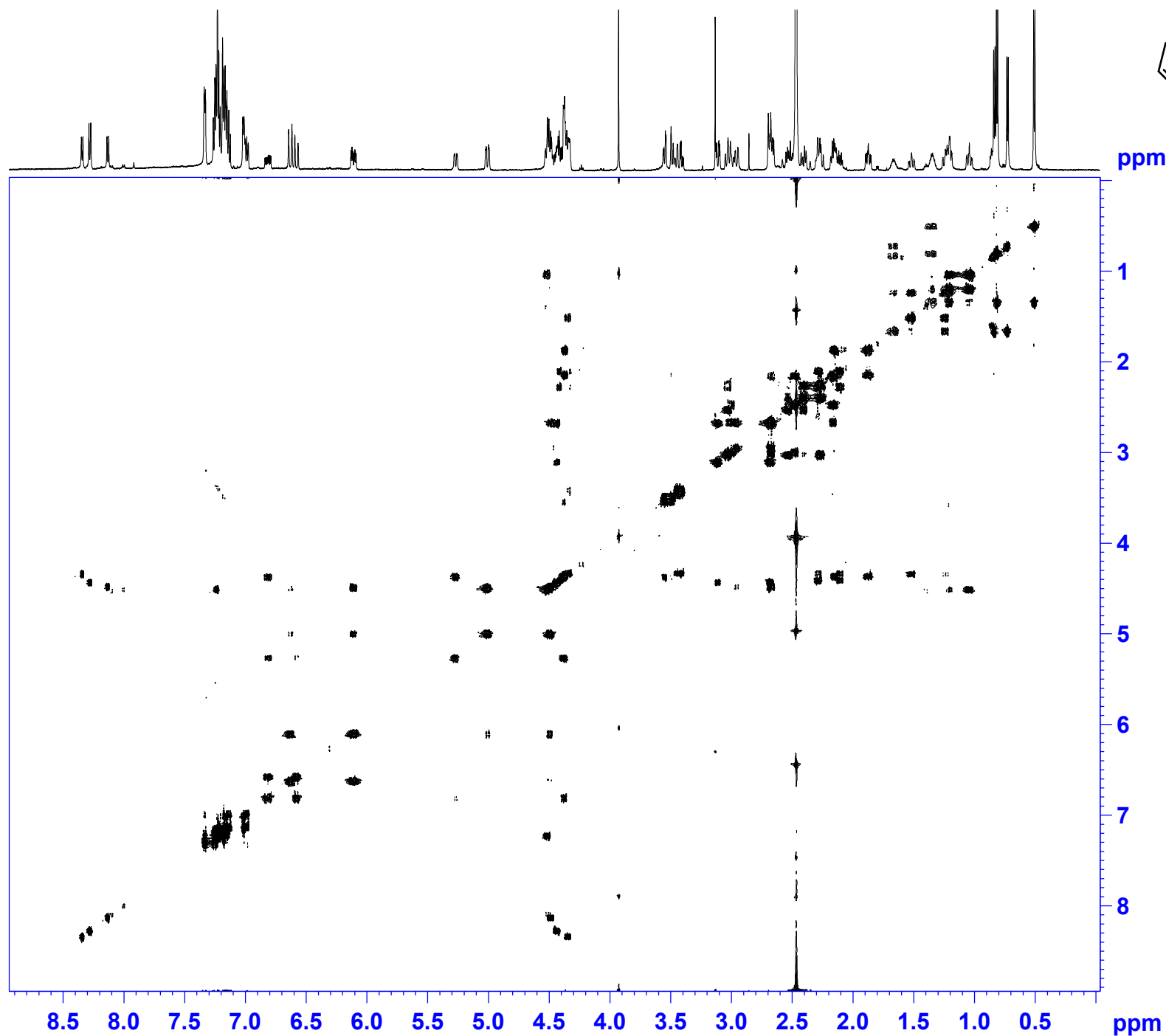
Current Data Parameters
NAME KL-5-12_AV500
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120821
Time 17.22
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 202.91
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PLW1 13.5000000 W
SF01 500.1330008 MHz

F2 - Processing parameters
SI 65536
SF 500.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



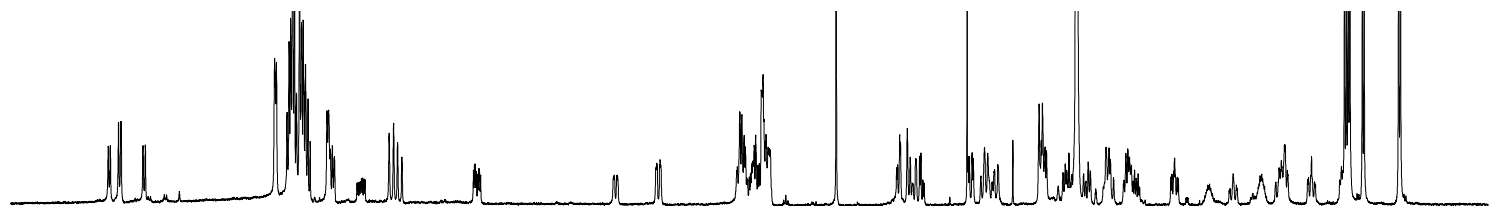


Current Data Parameters
 NAME K1-5-12
 EXPNO 3
 PROCNO 1

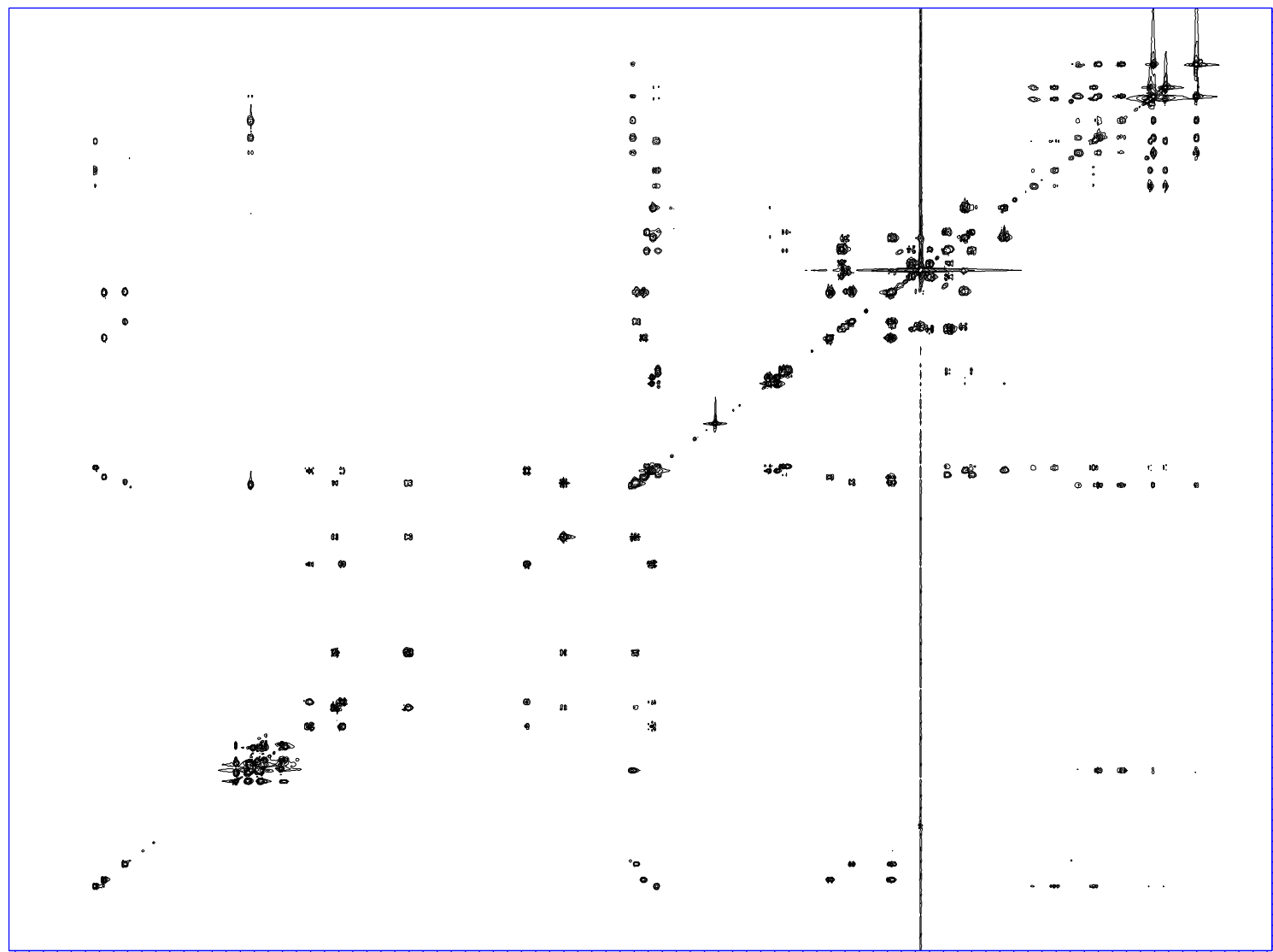
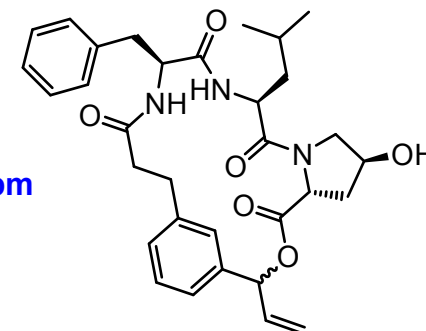
F1 - Acquisition parameters
 TD 256
 SFO1 600.1327 MHz
 FIDRES 21.046595 Hz
 SW 8.978 ppm
 FnMODE States-TPPI

F2 - Processing parameters
 SI 2048
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 States-TPPI
 SF 600.1300273 MHz
 WDW TRAP
 SSB 2
 LB 0 Hz
 GB 0



ppm



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

ppm

1

2

3

4

5

6

7

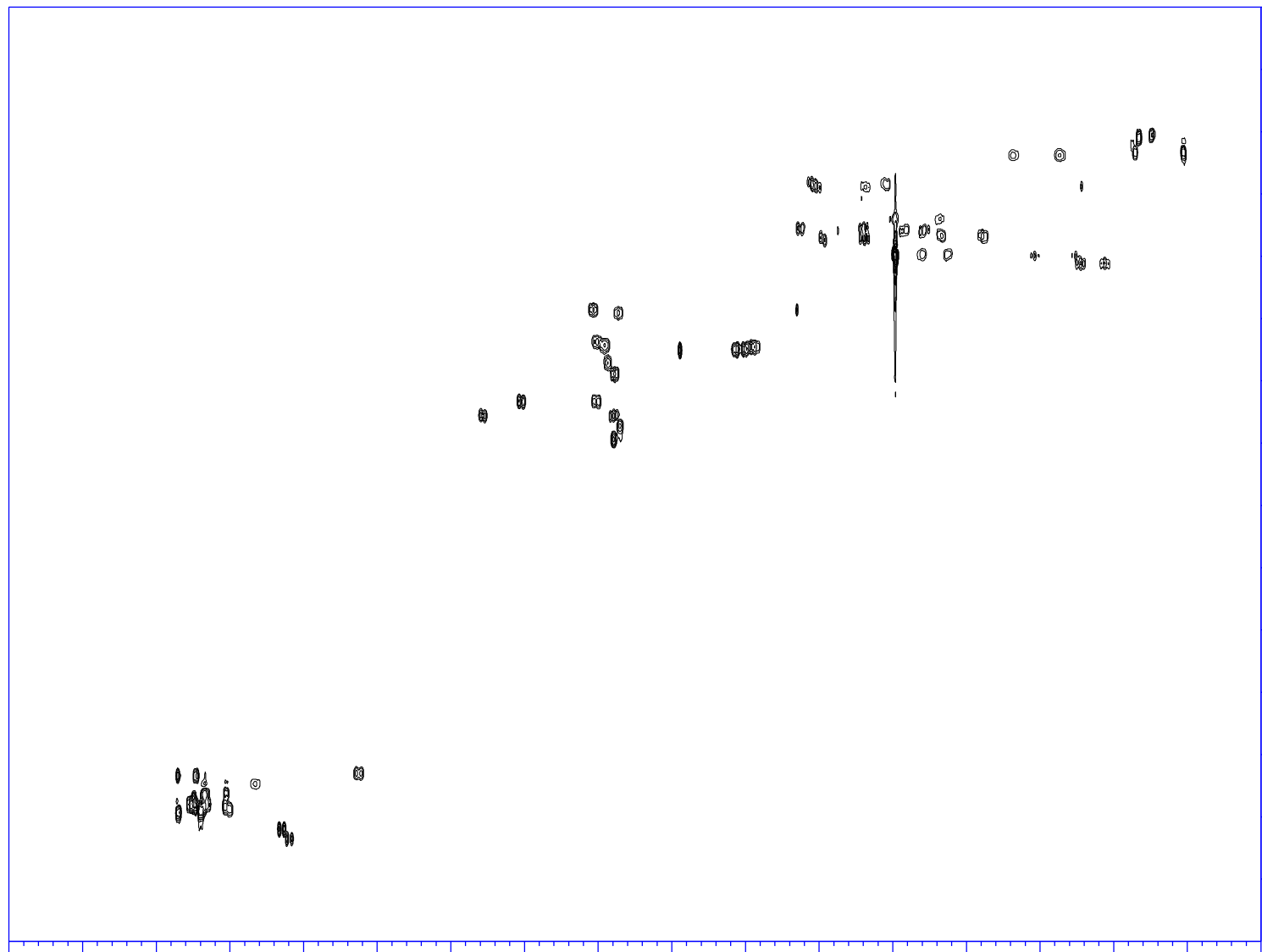
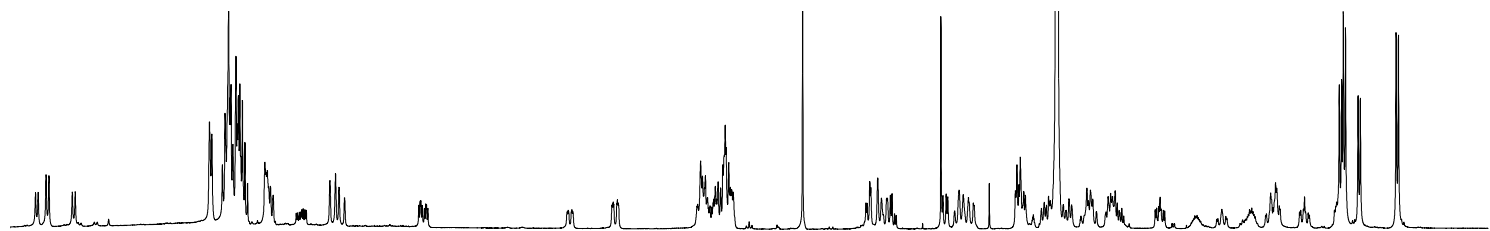
8

Current Data Parameters
 NAME K1-5-12
 EXPNO 4
 PROCNO 1

F1 - Acquisition parameters
 TD 600
 SFO1 600.1327 MHz
 FIDRES 10.602203 Hz
 SW 10.600 ppm
 FnMODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 echo-antiecho
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0



ppm

20

40

60

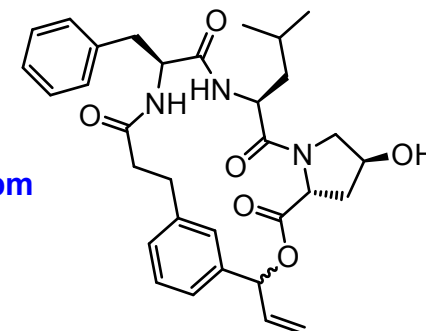
80

100

120

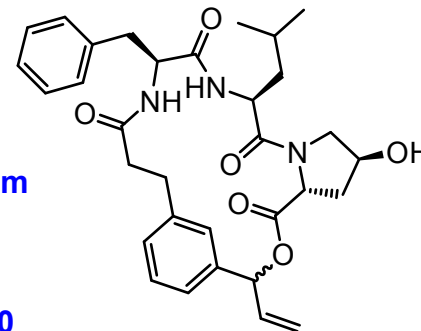
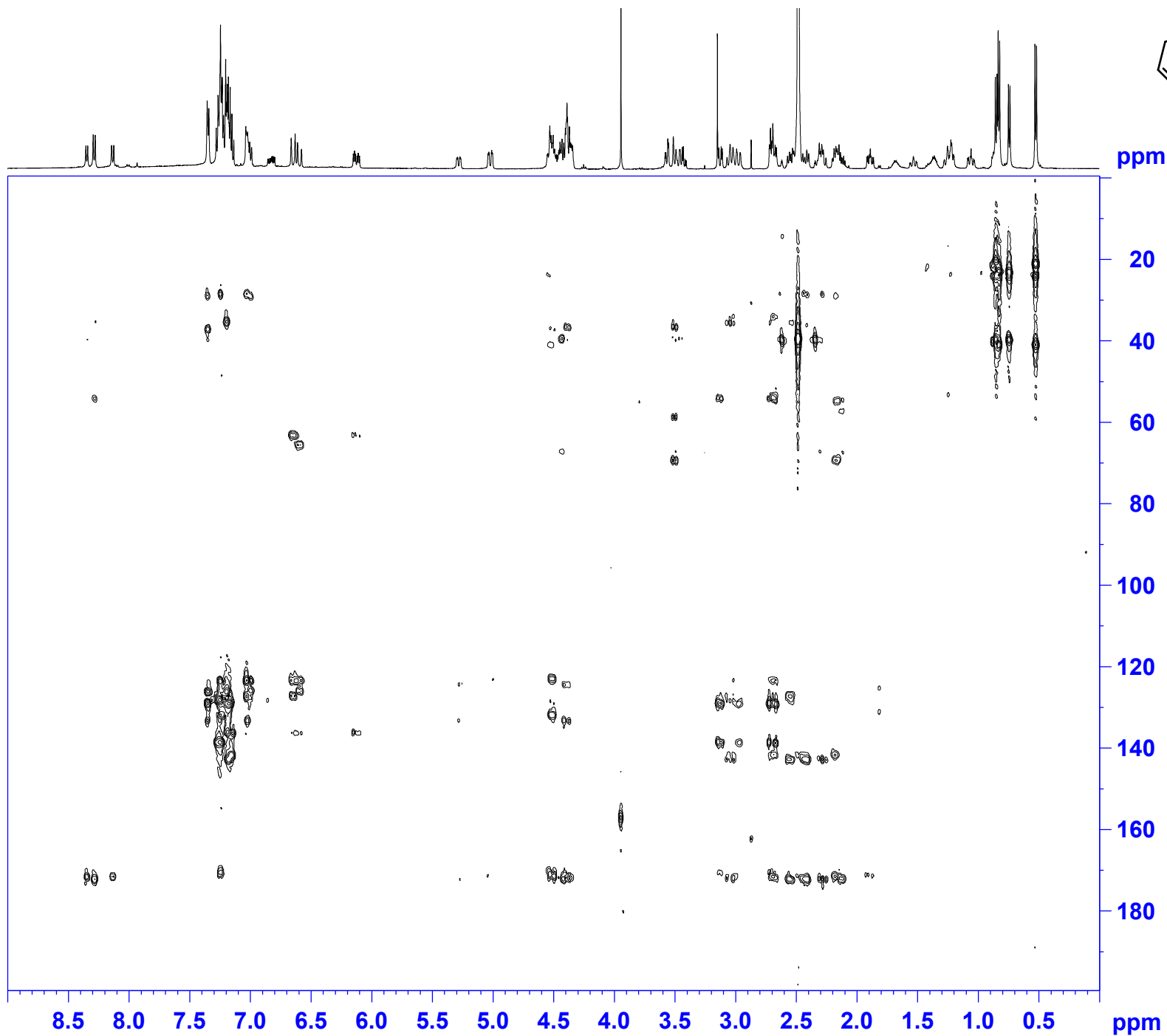
140

ppm



Current Data Parameters
 NAME KL-5-12_AV500
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120821
 Time 17.24
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hsqcedetgp
 TD 2048
 SOLVENT DMSO
 NS 4
 DS 16
 SWH 5000.000 H:
 FIDRES 2.441406 H:
 AQ 0.2048000 s:
 RG 202.91
 DW 100.000 u:
 DE 10.00 u:
 TE 298.0 K
 CNST2 145.0000000
 d0 0.00000300 s:
 D1 1.50000000 s:
 d4 0.00172414 s:
 d11 0.03000000 s:
 d13 0.00000400 s:
 D16 0.00020000 s:
 D21 0.00345000 s:
 DELTA 0.00222400 s:
 DELTA1 0.00071614 s:
 in0 0 sec
 ST1CNT 128
 ZGOPTNS
 d0orig 0.00000300 s:
 phlloop 0
 tllloop 0
 SFO1 500.1325007 M:
 NUC1 1H
 P1 10.00 u:
 p2 20.00 u:
 P28 0 usec
 PLW1 13.50000000 W
 SFO2 125.7678496 M:
 NUC2 13C
 CPDPRG[2] garp
 P3 9.63 u:
 p4 19.26 u:
 PCPD2 70.00 u:
 PT.M? 23 n1399994 W



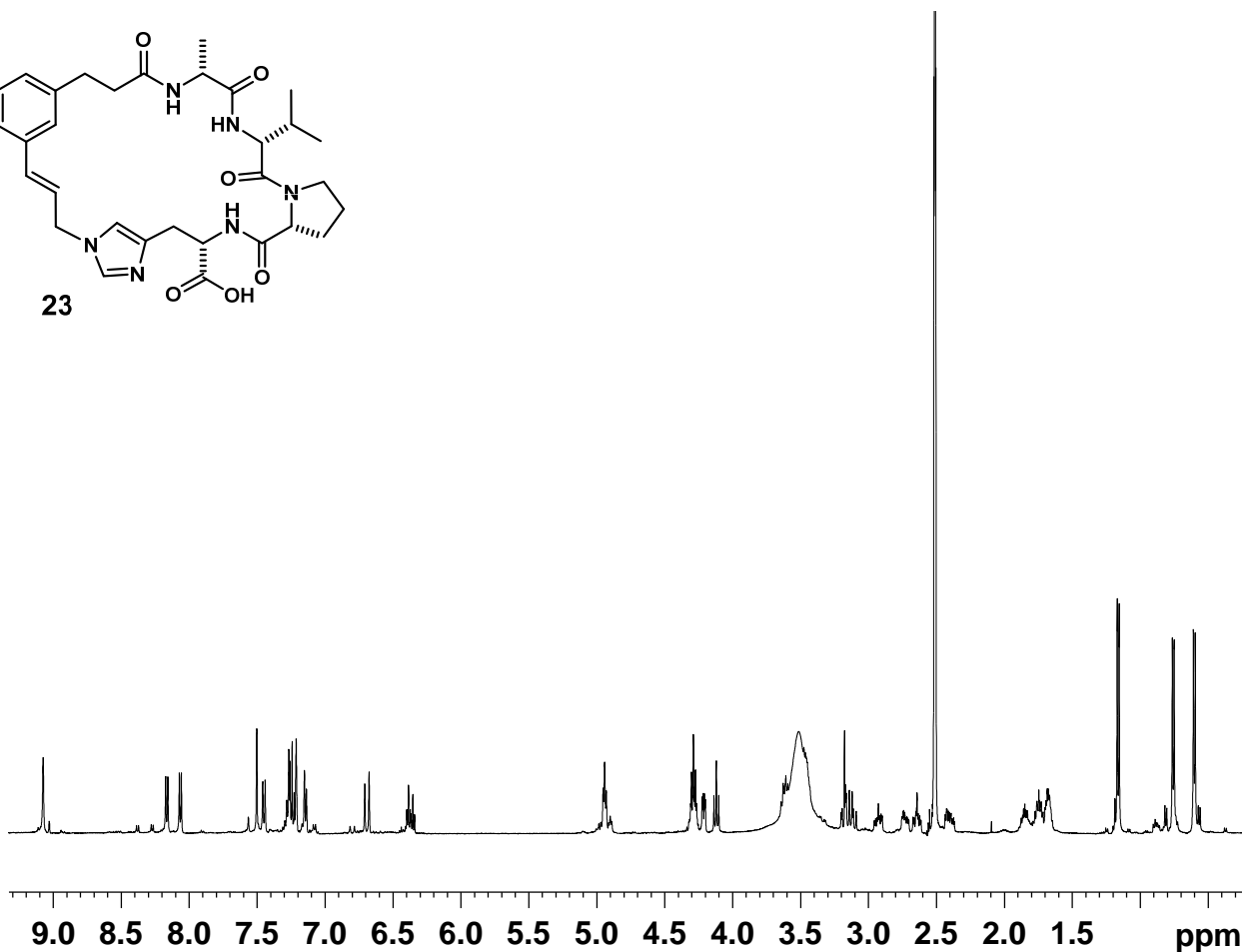
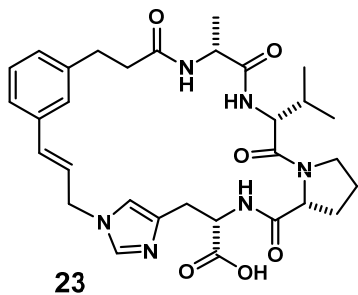
Current Data Parameters
 NAME KL-5-12_AV500
 EXPNO 3
 PROCNO 1

F1 - Acquisition parameters
 TD 256
 SFO1 125.7704 MHz
 FIDRES 98.257607 Hz
 SW 199.999 ppm
 FnmODE QF

F2 - Processing parameters
 SI 2048
 SF 500.1300135 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 QF
 SF 125.7578472 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

Cyclic-Ala-Val-Pro-His-OH (23):



```

Current Data Parameters
NAME      KL-4-183_F14_ICON
EXPNO     1
PROCNO    1

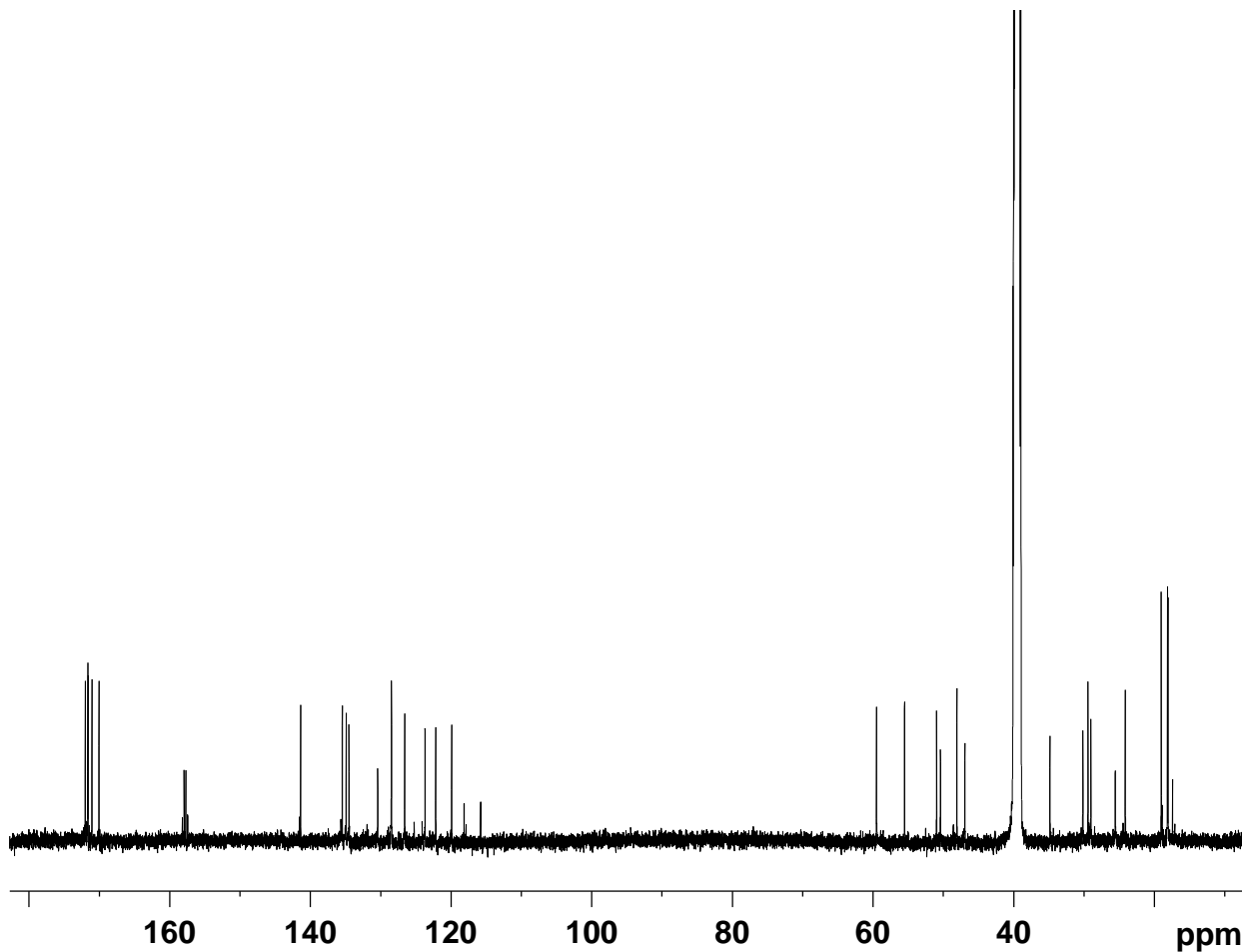
F2 - Acquisition Parameters
Date_     20120827
Time      20.16
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2767999 sec
RG         11
DW         50.000 usec
DE         10.00 usec
TE         298.0 K
D1         2.00000000 sec
TD0        1
    
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
PLW1     13.5000000 W
SFO1     500.1330008 MHz
    
```

```

F2 - Processing parameters
SI         65536
SF         500.1300000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

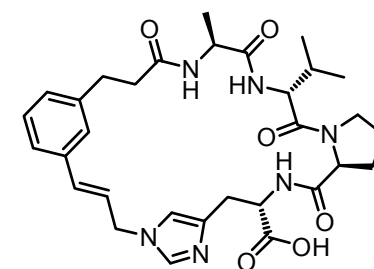
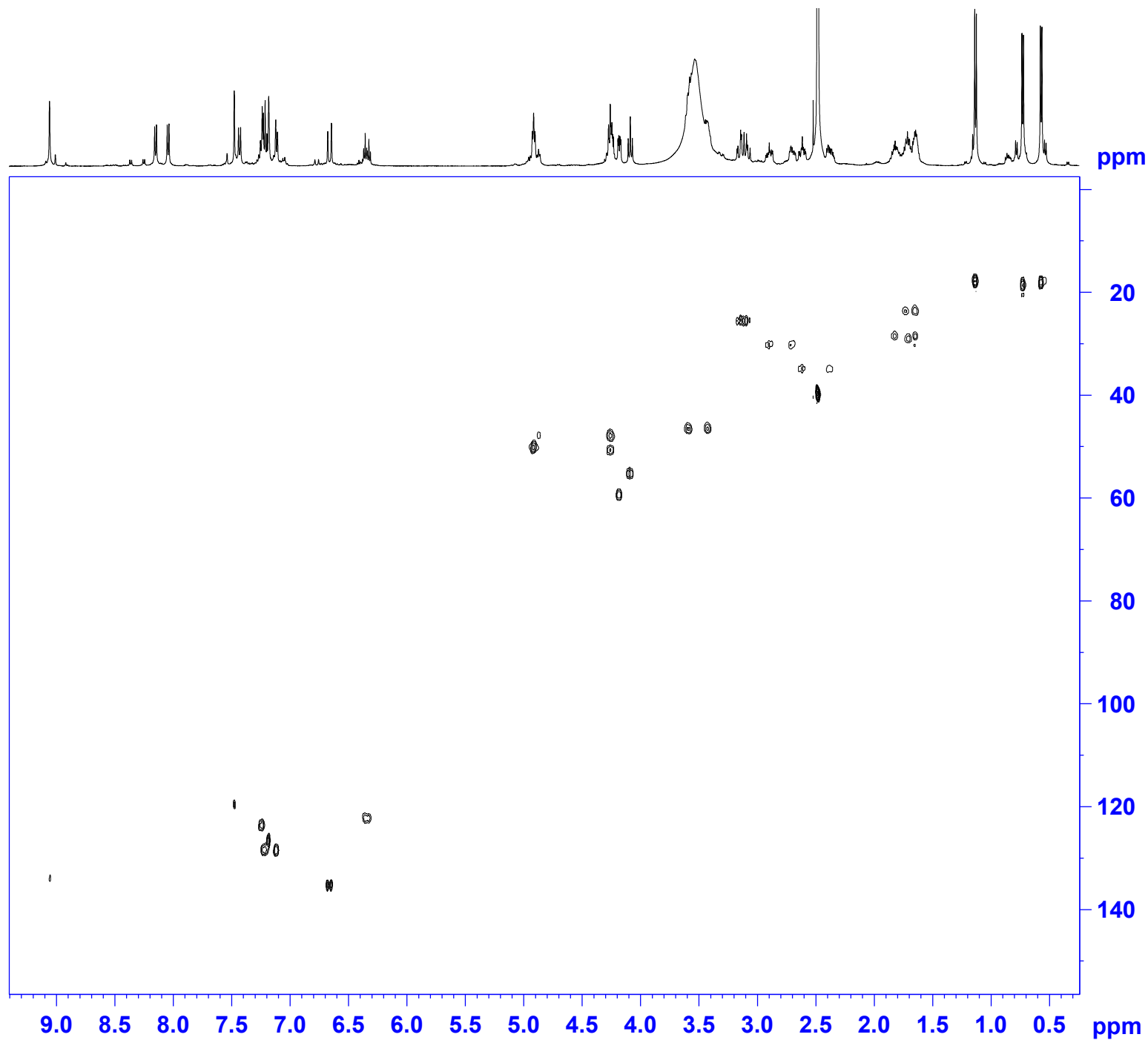


```

Current Data Parameters
NAME      KL-4-183_F14_ICON
EXPNO     2
PROCNO    1
    
```

```

F2 - Processing parameters
SI         131072
SF         125.7578519 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

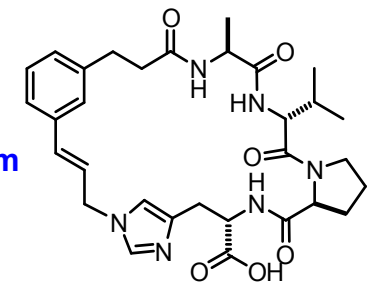
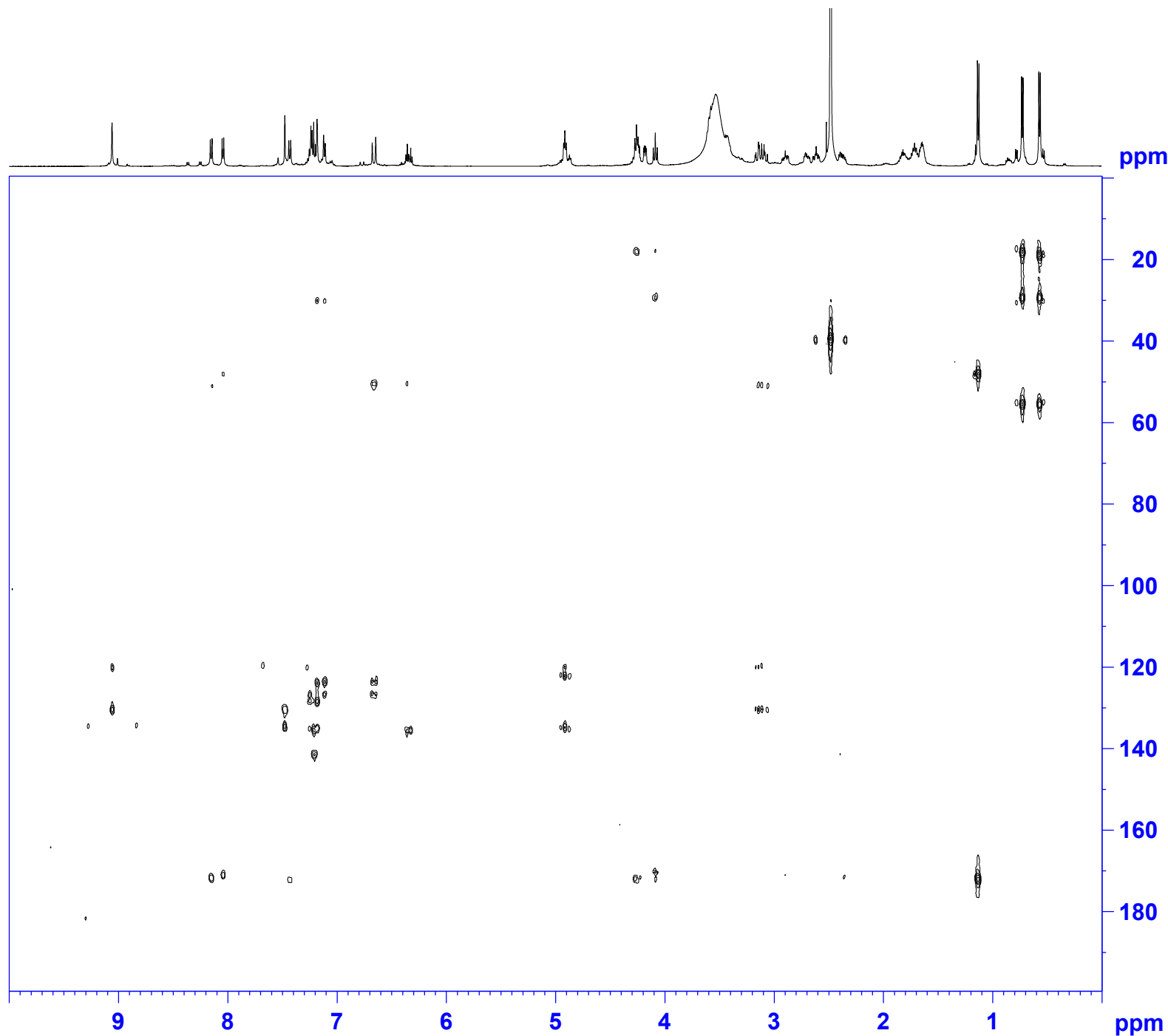


Current Data Parameters
 NAME KL-4-183_F14
 EXPNO 5
 PROCNO 1

F1 - Acquisition parameters
 TD 256
 SFO1 125.7678 MHz
 FIDRES 98.255890 Hz
 SW 200.000 ppm
 FnmODE Echo-Antiecho

F2 - Processing parameters
 SI 2048
 SF 500.1300135 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

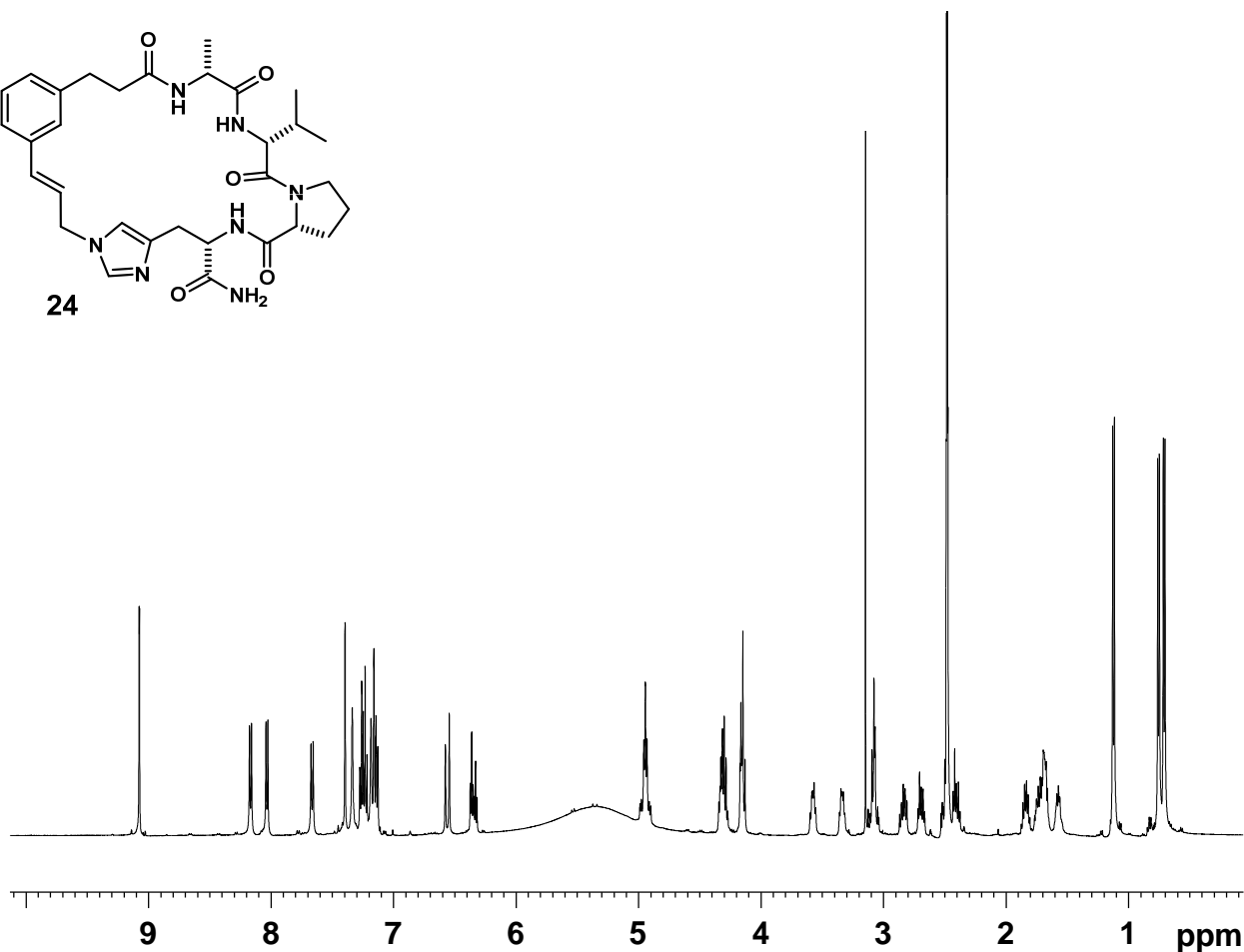
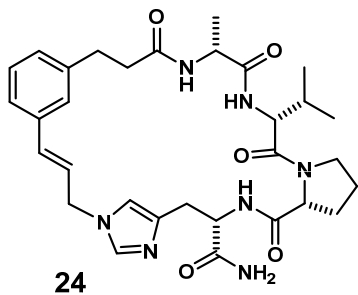
F1 - Processing parameters
 SI 2048
 MC2 echo-antiecho
 SF 125.7578472 MHz
 WDW TRAP
 SSB 2
 LB 0 Hz
 GB 0



Current Data Parameters
 NAME KL-4-183_F14
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120731
 Time 12.18
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hmhbcgpl2ndqf
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 44.31
 DW 83.200 u:
 DE 10.00 u:
 TE 296.0 K
 CNST6 120.0000000
 CNST7 160.0000000
 CNST13 7.0000000
 d0 0.00000300 s:
 D1 2.00000000 s:
 d6 0.07142857 s:
 D16 0.00020000 s:
 DELTA1 0.00296667 s:
 DELTA2 0.00192500 s:
 DELTA3 0.07022458 s:
 in0 0 sec
 ST1CNT 256
 d0orig 0.00000300 s:
 philloop 0
 tllloop 0
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 10.00 u:
 p2 20.00 u:
 PLW1 13.50000000 W
 SFO2 125.7703648 MHz
 NUC2 13C
 P3 9.63 u:
 PLW2 23.01399994 W
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPNAM[4] SMSQ10.100
 GPNAM[5] SMSQ10.100

Cyclic-Ala-Val-Pro-His-NH₂ (24):

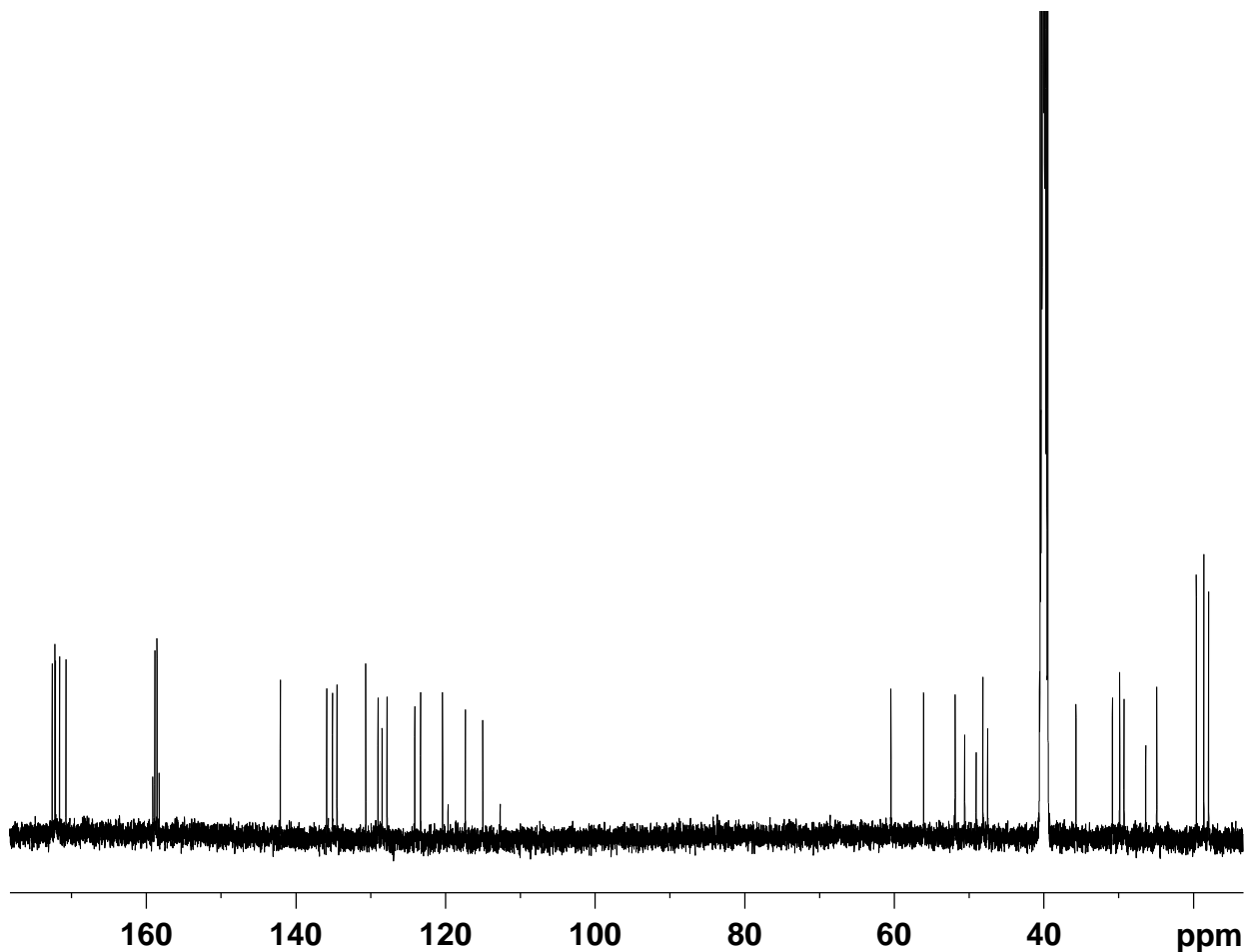


```
Current Data Parameters
NAME      KL-4-206A_F22
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20120731
Time      12.41
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2767999 sec
RG         202.91
DW         50.000 usec
DE         10.00 usec
TE         296.0 K
D1         2.00000000 sec
D11        1
TD0        1
```

```
===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
PLW1     13.5000000 W
SFO1     500.1330008 MHz
```

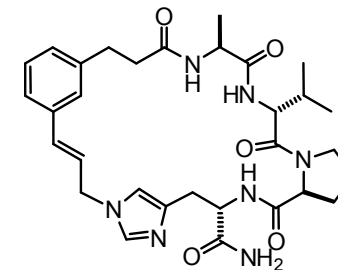
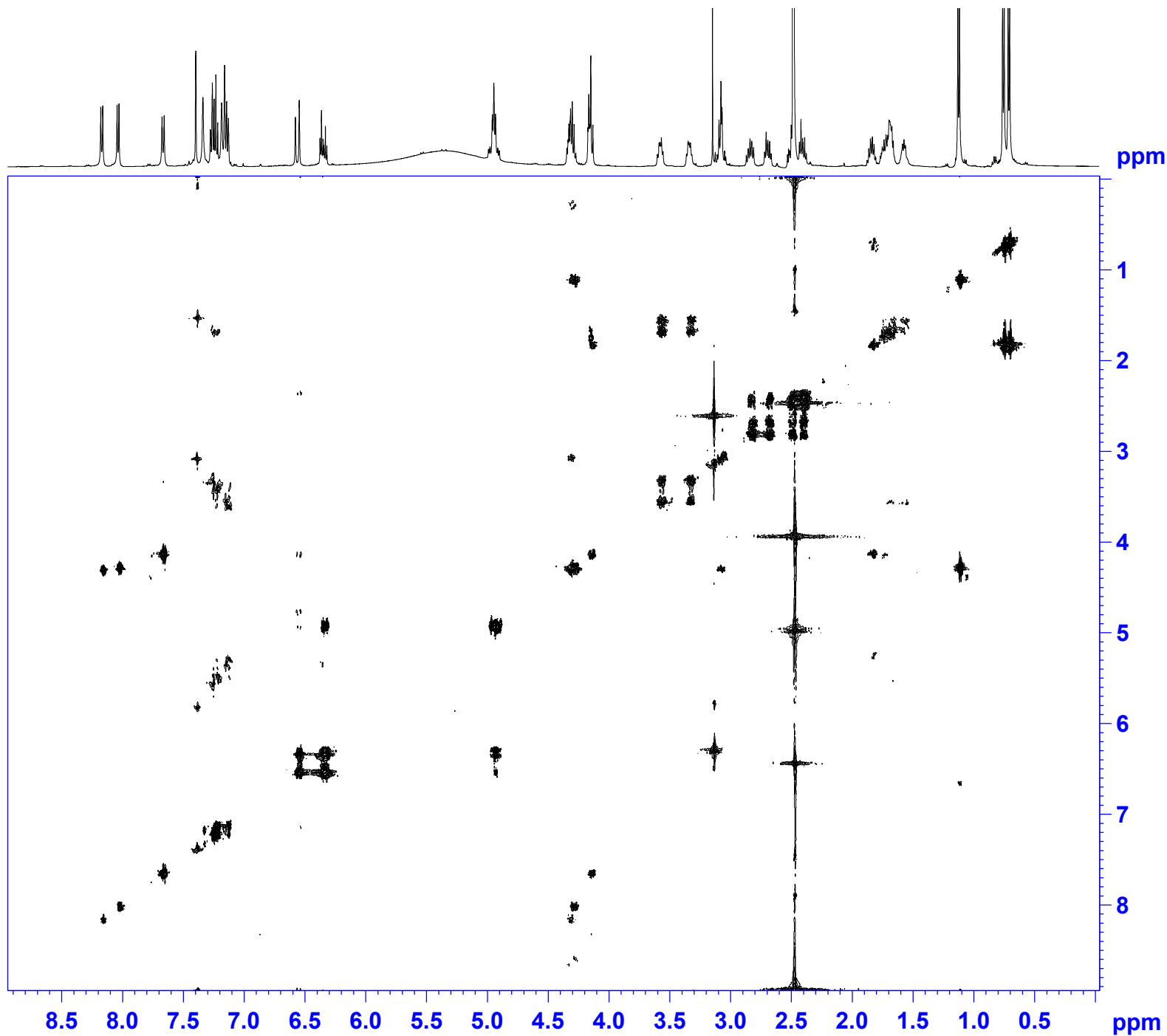
```
F2 - Processing parameters
SI        65536
SF        500.1300146 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```



```
Current Data Parameters
NAME      KL-4-206A_F22
EXPNO     5
PROCNO    1
```

```
F2 - Acquisition Parameters
Date_     20120821
Time      19.30
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         128
DS         2
SWH        31250.000 Hz
FIDRES     0.476837 Hz
AQ         1.0485760 sec
RG         202.91
DW         16.000 usec
DE         18.00 usec
TE         298.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
SFO1     125.7722511 MHz
NUC1      13C
P1        9.63 usec
PLW1     23.00000000 W
SFO2     500.1330008 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     80.00 usec
PLW2     13.50000000 W
PLW12    0.21094000 W
PLW13    0.13500001 W
```

```
F2 - Processing parameters
SI        131072
SF        125.7577892 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

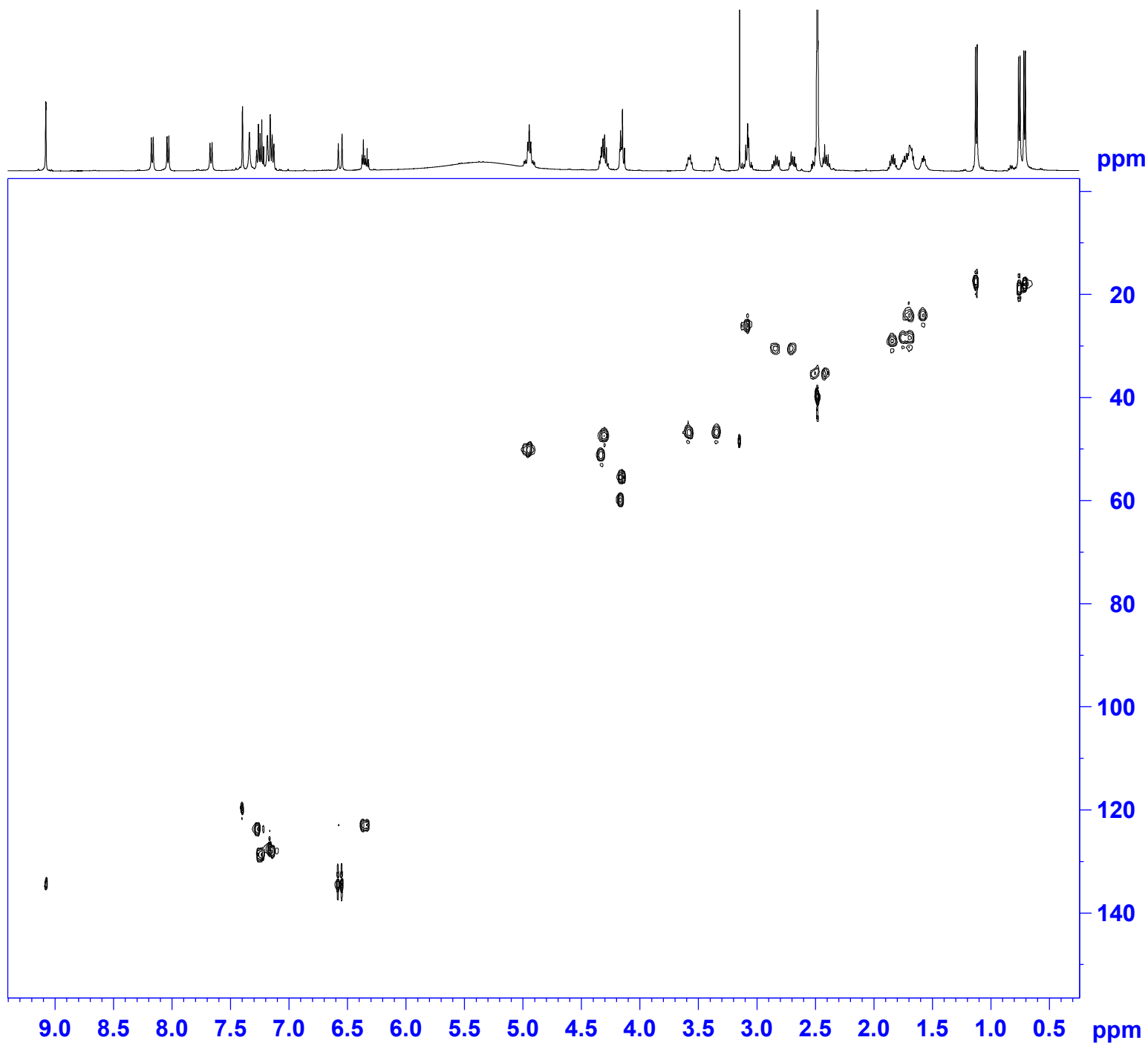


Current Data Parameters
 NAME KL-4-206A_F22
 EXPNO 3
 PROCNO 1

F1 - Acquisition parameters
 TD 256
 SFO1 600.1327 MHz
 FIDRES 21.046595 Hz
 SW 8.978 ppm
 FnmODE States-TPPI

F2 - Processing parameters
 SI 2048
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 States-TPPI
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

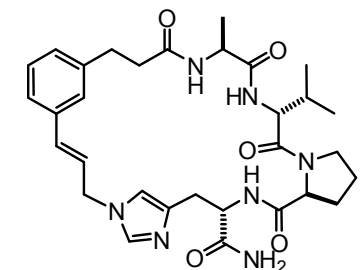
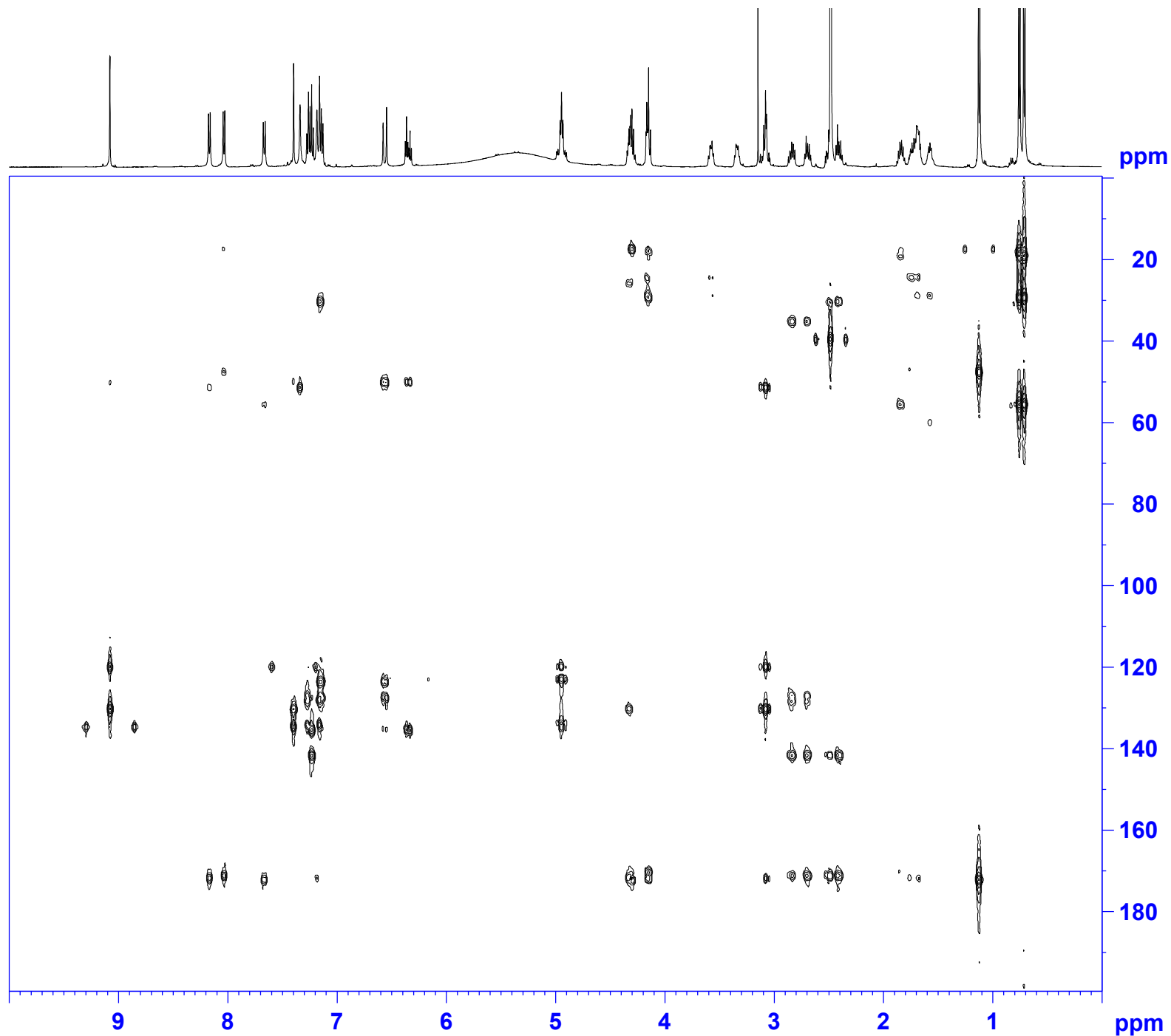


Current Data Parameters
 NAME KL-4-206A_F22
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120731
 Time_ 12.41
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 202.91
 DW 50.000 usec
 DE 10.00 usec
 TE 296.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PLW1 13.5000000 W
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



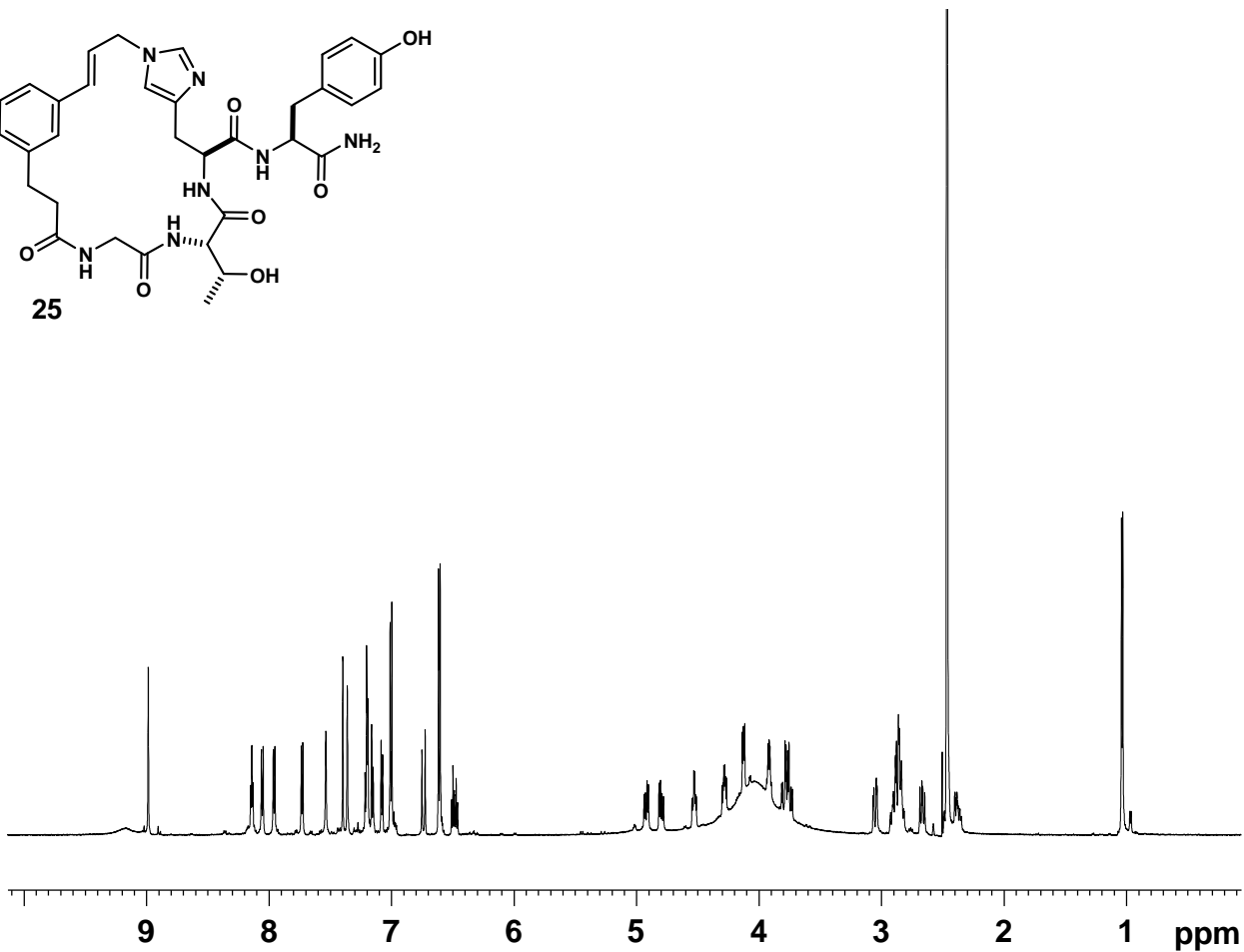
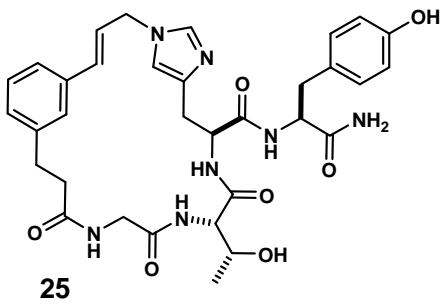
Current Data Parameters
 NAME KL-4-206A_F22
 EXPNO 2
 PROCNO 1

F1 - Acquisition parameters
 TD 220
 SFO1 125.7704 MHz
 FIDRES 114.336121 Hz
 SW 199.999 ppm
 FnMODE QF

F2 - Processing parameters
 SI 2048
 SF 500.1300135 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 QF
 SF 125.7578472 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

Cyclic-Gly-Thr-His-Tyr-NH₂ (25):



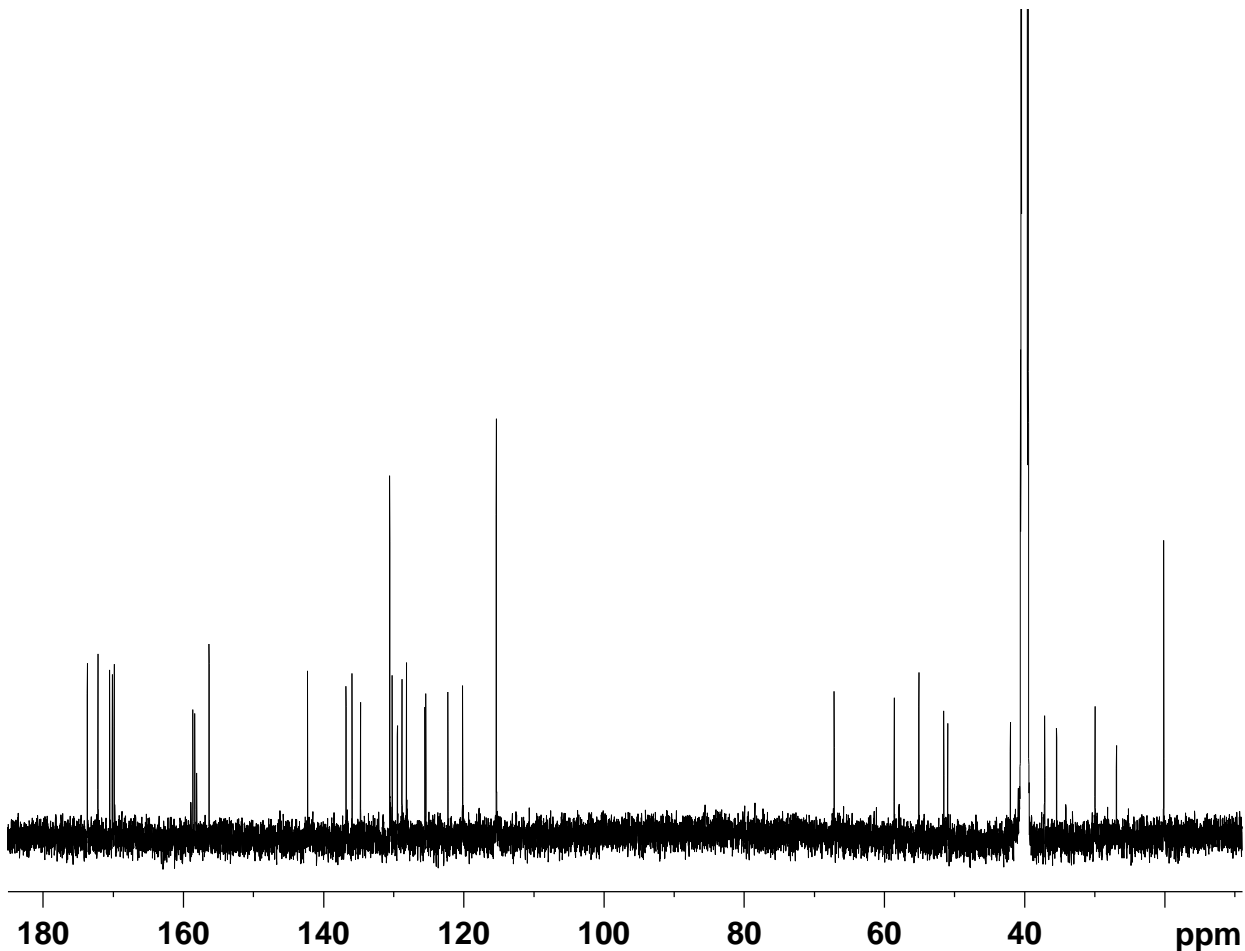
```

Current Data Parameters
NAME      His_A2_F17
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20121207
Time      17.19
INSTRUM   av600
PROBHD    5 mm TBI5
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         0
SWH        12376.237 Hz
FIDRES     0.188846 Hz
AQ         2.6476543 sec
RG         256
DW         40.400 usec
DE         6.50 usec
TE         294.0 K
D1         2.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         9.10 usec
PL1        -2.00 dB
PL1W       39.81071854 W
SFO1       600.1336008 MHz

F2 - Processing parameters
SI         65536
SF         600.1300273 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



```

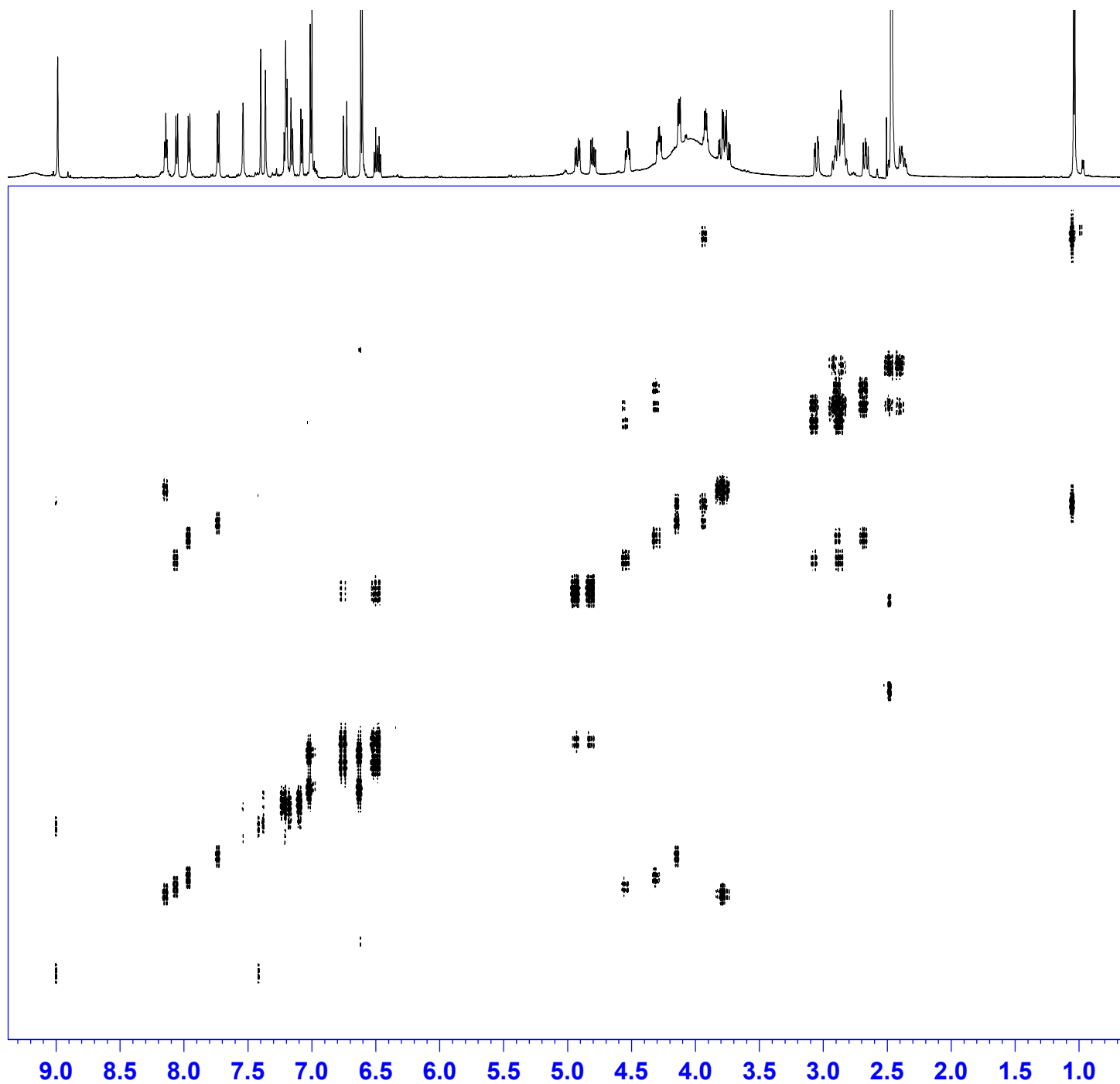
Current Data Parameters
NAME      His_A2_F17
EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
Date_     20121220
Time      17.18
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         2
SWH        31250.000 Hz
FIDRES     0.476837 Hz
AQ         1.0485760 sec
RG         202.91
DW         16.000 usec
DE         18.00 usec
TE         298.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1       125.7722511 MHz
NUC1        13C
P1         9.63 usec
PLW1       23.00000000 W

===== CHANNEL f2 =====
SFO2       500.1330008 MHz
NUC2        1H
CPDPRG[2   waltz16
PCPD2       80.00 usec
PLW2        13.50000000 W
PLW12       0.21094000 W
PLW13       0.13500001 W

F2 - Processing parameters
SI         131072
SF         125.7577892 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```



ppm

0

1

2

3

4

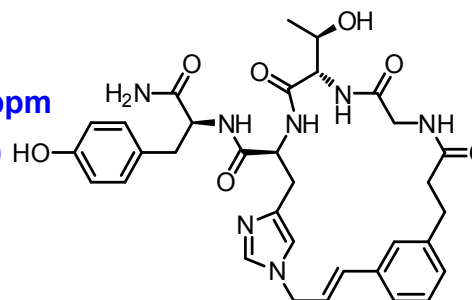
5

6

7

8

ppm



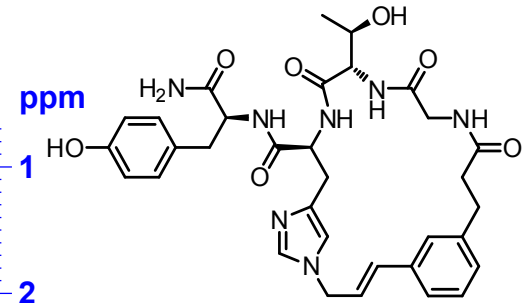
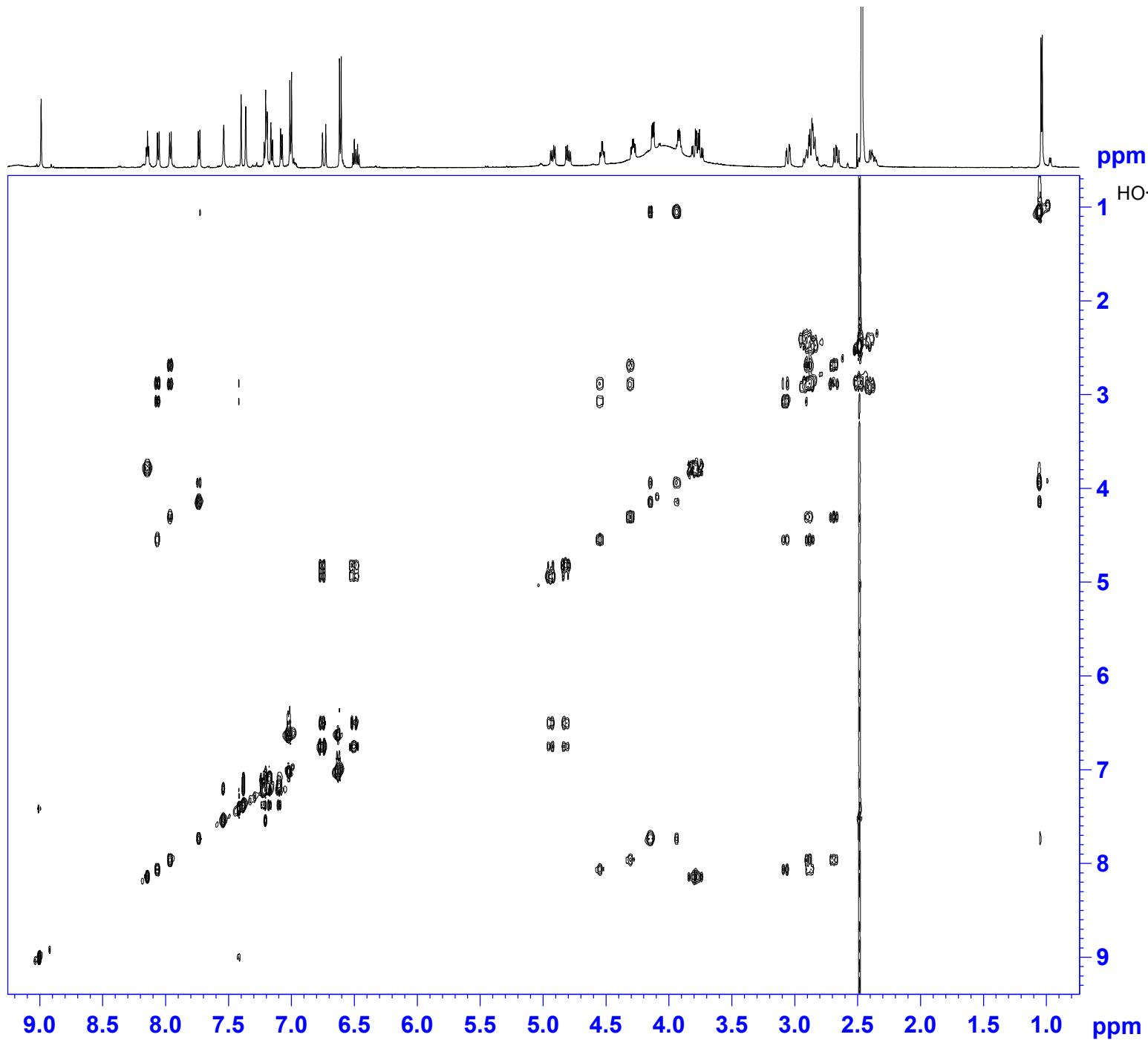
Current Data Parameters
 NAME His_A2_F17
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20121220
 Time 17.48
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG cosygmfph
 TD 4096
 SOLVENT DMSO
 NS 2
 DS 8
 SWH 5498.534 H:
 FIDRES 1.342415 H:
 AQ 0.3724629 s:
 RG 202.91
 DW 90.933 u:
 DE 10.00 u:
 TE 298.0 K
 D0 0.00007817 s:
 D1 2.00000000 s:
 D13 0.00000400 s:
 D16 0.00020000 s:
 IN0 0.00018180 s:

===== CHANNEL f1 =====
 SFO1 500.1327507 M:
 NUC1 1H
 P1 10.00 u:
 P2 20.00 u:
 PLW1 13.50000000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPZ1 10.00 %
 GPZ2 20.00 %
 P16 1000.00 u:

F1 - Acquisition parameters:
 TD 256
 SFO1 500.1328 M:
 FIDRES 21.486525 H:
 SW 10.998 p:

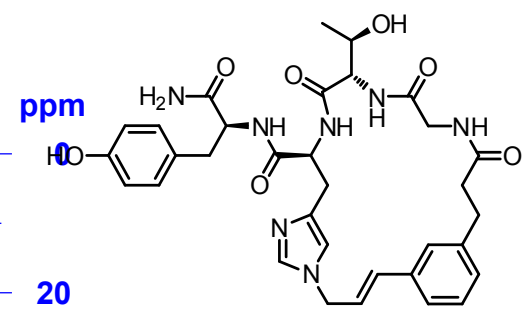
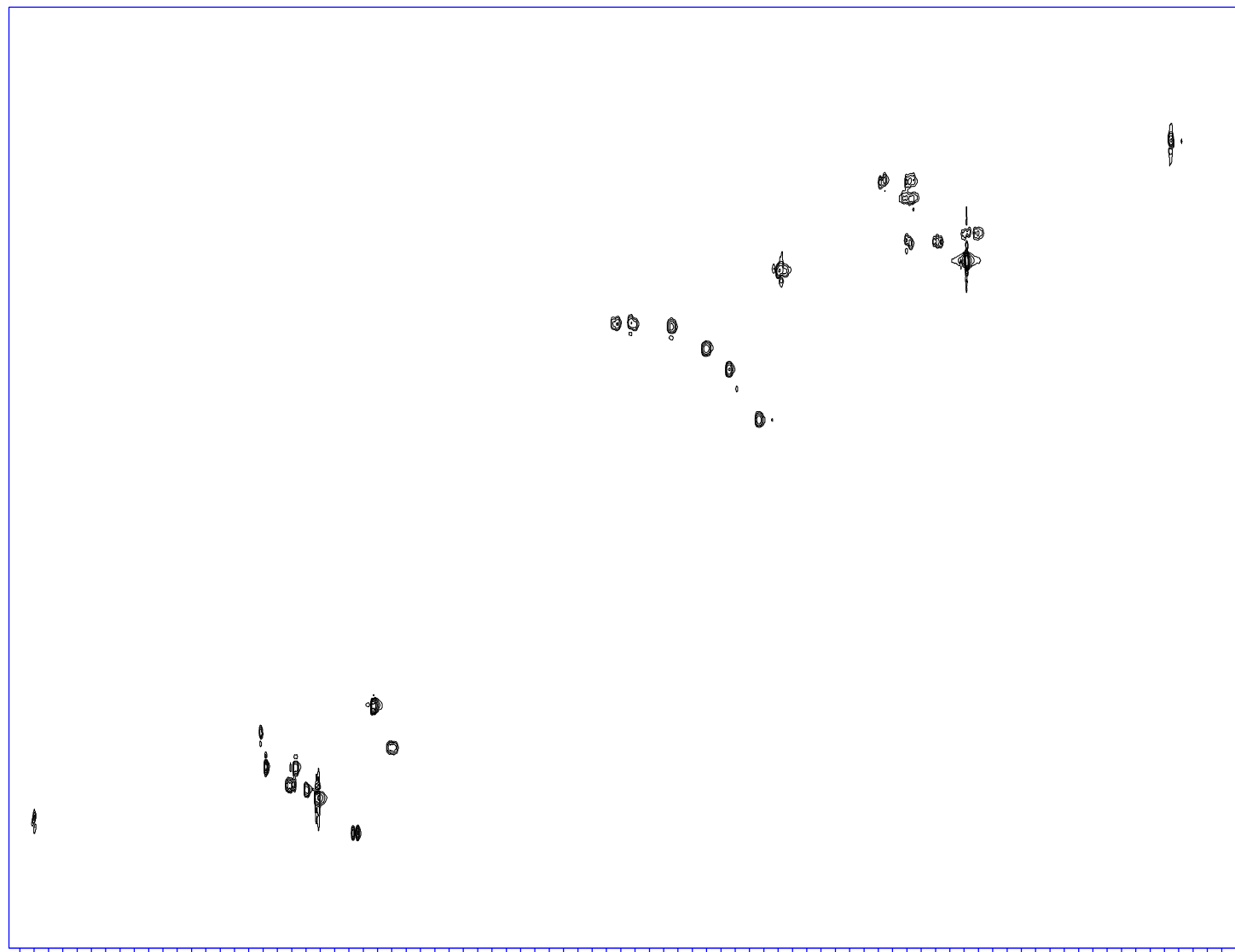
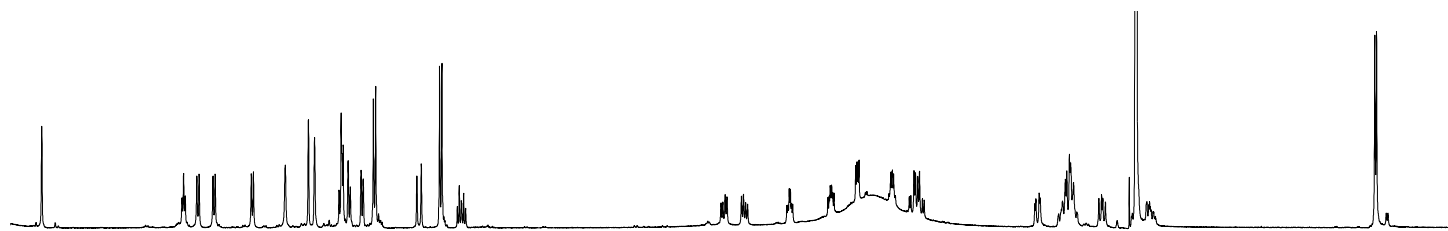


Current Data Parameters
 NAME His_A2_F17
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121208
 Time 12.00
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG mlevetgp.js
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 8
 SWH 5000.000 H:
 FIDRES 2.441406 H:
 AQ 0.2048000 s:
 RG 37.94
 DW 100.000 u:
 DE 10.00 u:
 TE 298.0 K
 D0 0.00000300 s:
 D1 2.00000000 s:
 D9 0.06000000 s:
 D11 0.03000000 s:
 D12 0.00002000 s:
 D16 0.00020000 s:
 IN0 0.00020000 s:
 L1 24

===== CHANNEL f1 =====
 SFO1 500.1325007 MHz
 NUC1 1H
 P1 10.00 u:
 P2 20.00 u:
 P5 26.68 u:
 P6 40.00 u:
 P7 80.00 u:
 P17 2500.00 u:
 PLW1 13.5000000 W
 PLW10 0.84375000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SINE.100
 GPNAM[2] SINE.100
 GPZ1 30.00 %



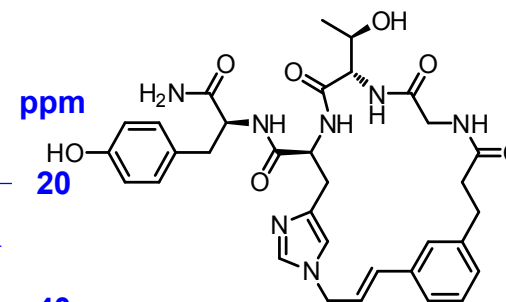
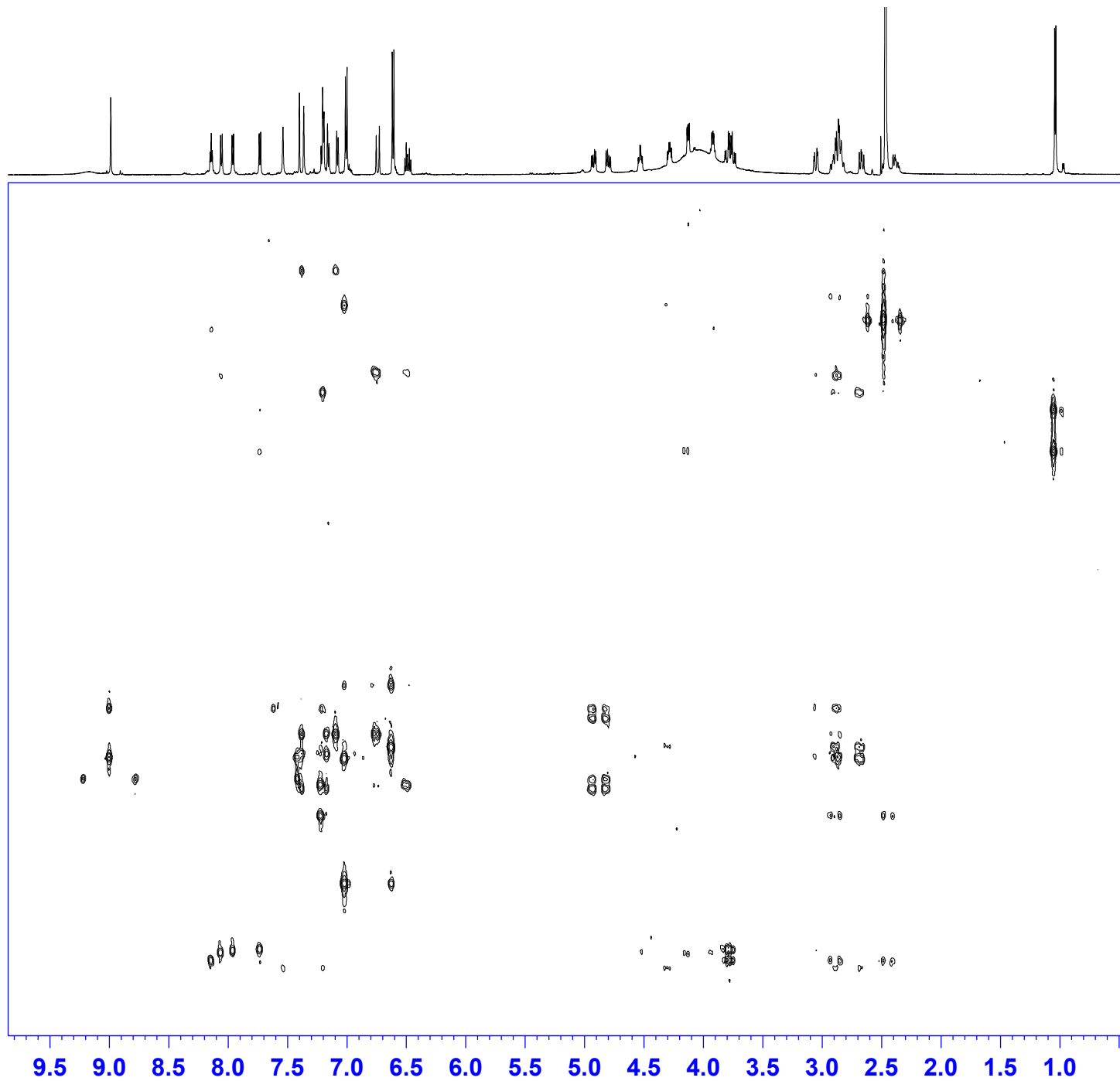
Current Data Parameters
 NAME His_A2_F17
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20121220
 Time 17.19
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hsqcedetgp
 TD 2048
 SOLVENT DMSO
 NS 4
 DS 16
 SWH 5000.000 H:
 FIDRES 2.441406 H:
 AQ 0.2048000 s:
 RG 202.91
 DW 100.000 u:
 DE 10.00 u:
 TE 298.0 K
 CNST2 145.000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D4 0.00172414 s:
 D11 0.03000000 s:
 D13 0.00000400 s:
 D16 0.00020000 s:
 D21 0.00345000 s:
 IN0 0.00001990 s:
 ZGOPTNS

===== CHANNEL f1 =====
 SFO1 500.1325007 MHz
 NUC1 1H
 P1 10.00 u:
 P2 20.00 u:
 P28 0 usec
 PLW1 13.50000000 W

===== CHANNEL f2 =====
 SFO2 125.7678496 MHz
 NUC2 13C
 CPDPRG[2] garp
 P3 9.63 u:
 P4 19.26 u:

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm



Current Data Parameters
 NAME His_A2_F17
 EXPNO 5
 PROCNO 1

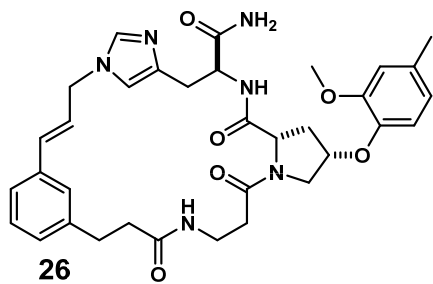
F2 - Acquisition Parameters
 Date_ 20121208
 Time 12.20
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 202.91
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D6 0.07142857 s:
 D16 0.00020000 s:
 IN0 0.00001990 s:

===== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 10.00 u:
 P2 20.00 u:
 PLW1 13.50000000 W

===== CHANNEL f2 =====
 SFO2 125.7703648 MHz
 NUC2 13C
 P3 9.63 u:
 PLW2 23.01399994 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100

Cyclic-β-Ala-Pro[4-(2-methoxy-4-methylphenoxy)]-His (26):

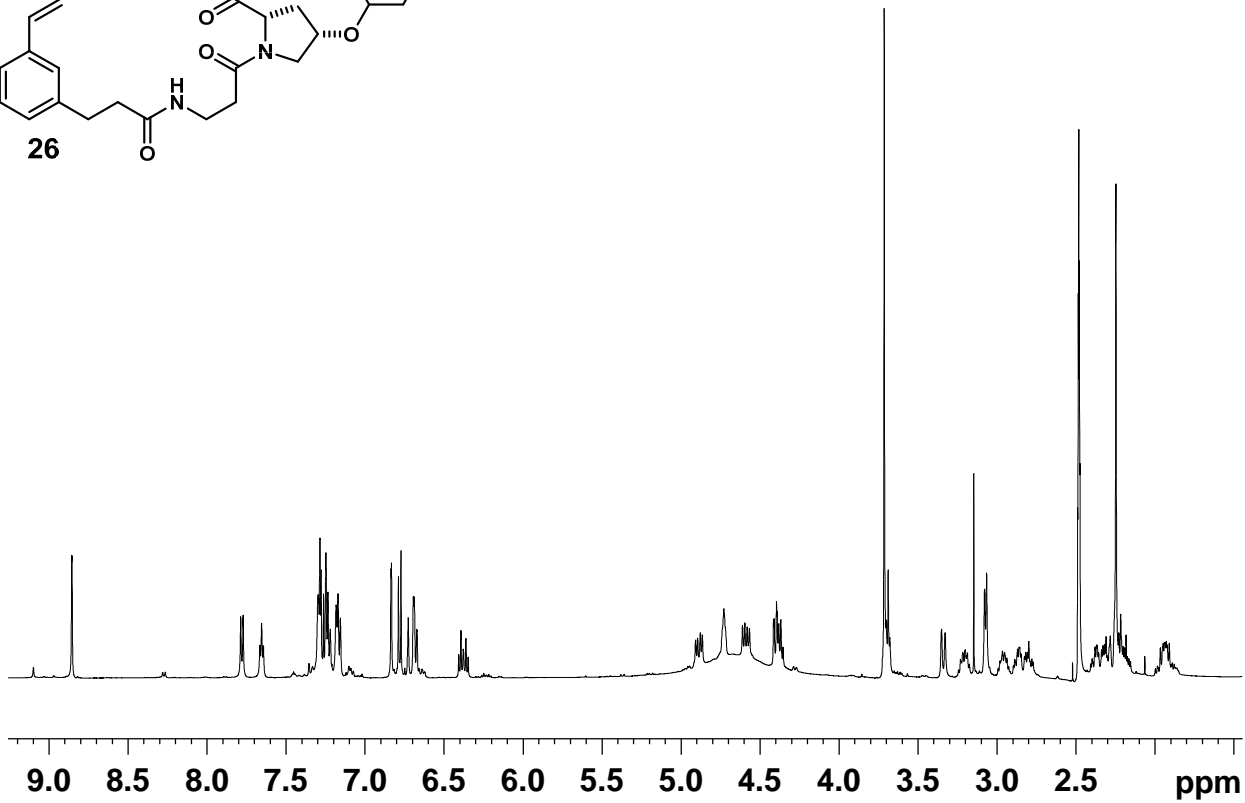


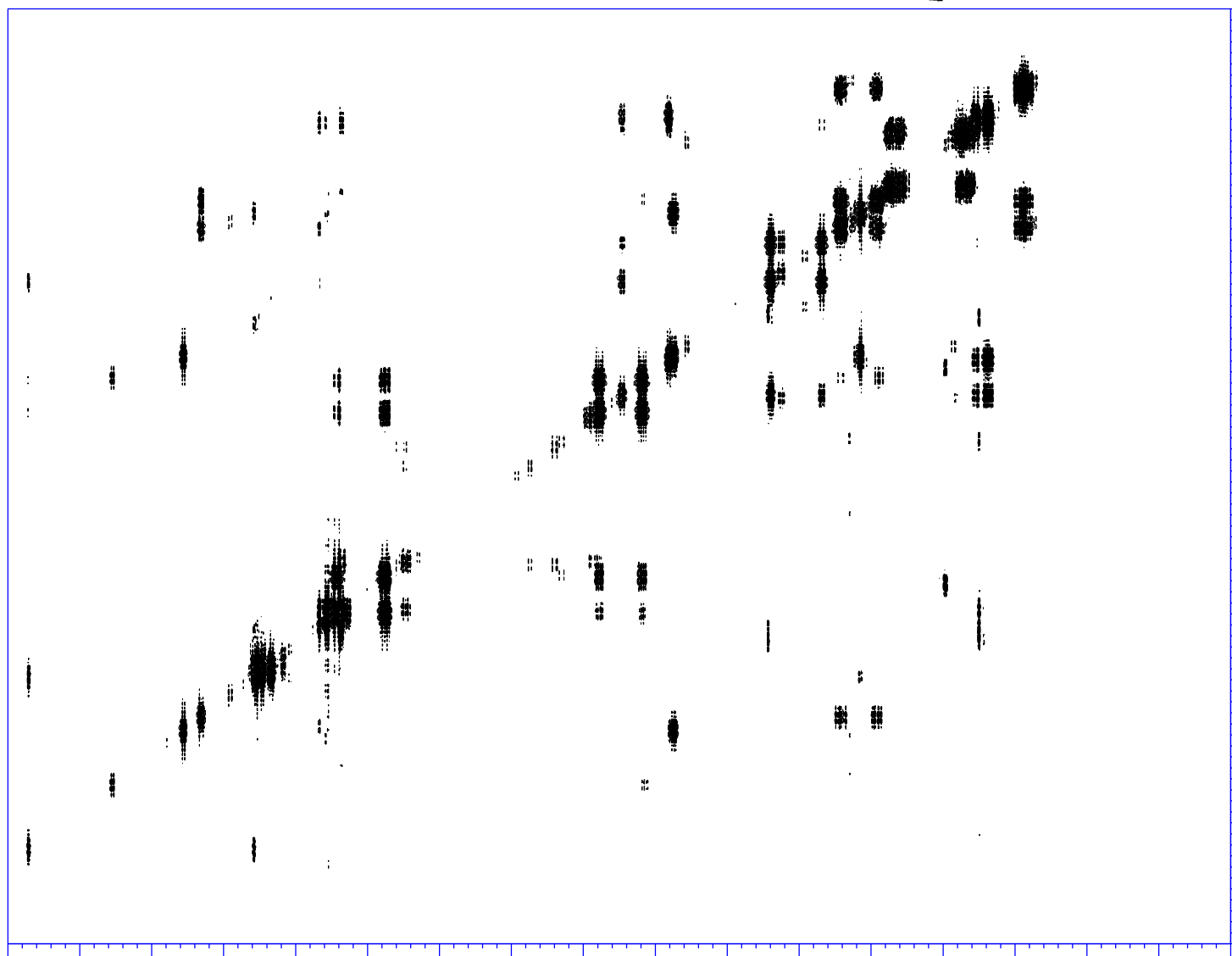
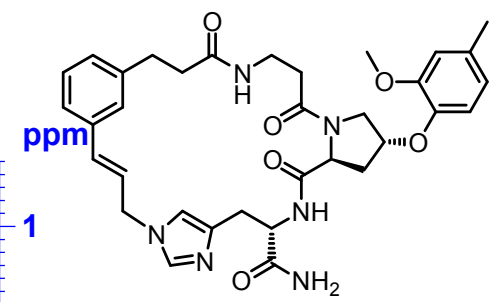
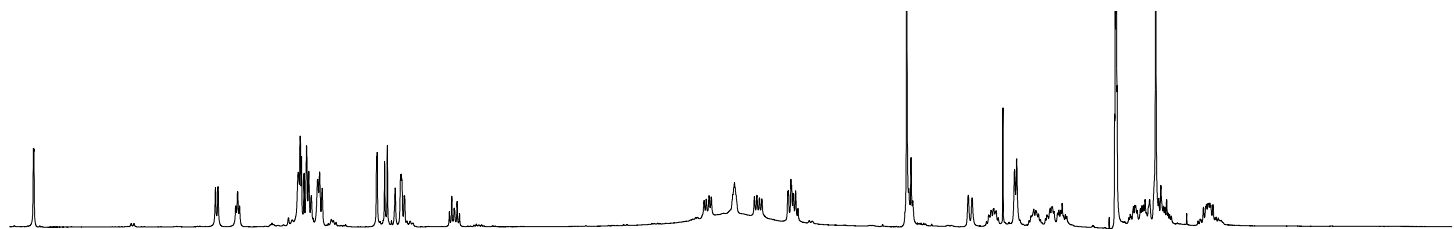
Current Data Parameters
NAME KL-4-221B_F7
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120731
Time 19.30
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 180.61
DW 50.000 usec
DE 10.00 usec
TE 296.0 K
D1 2.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PLW1 13.5000000 W
SF01 500.1330008 MHz

F2 - Processing parameters
SI 65536
SF 500.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

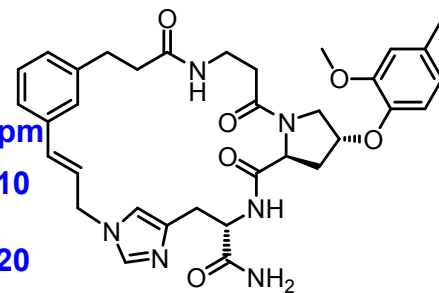
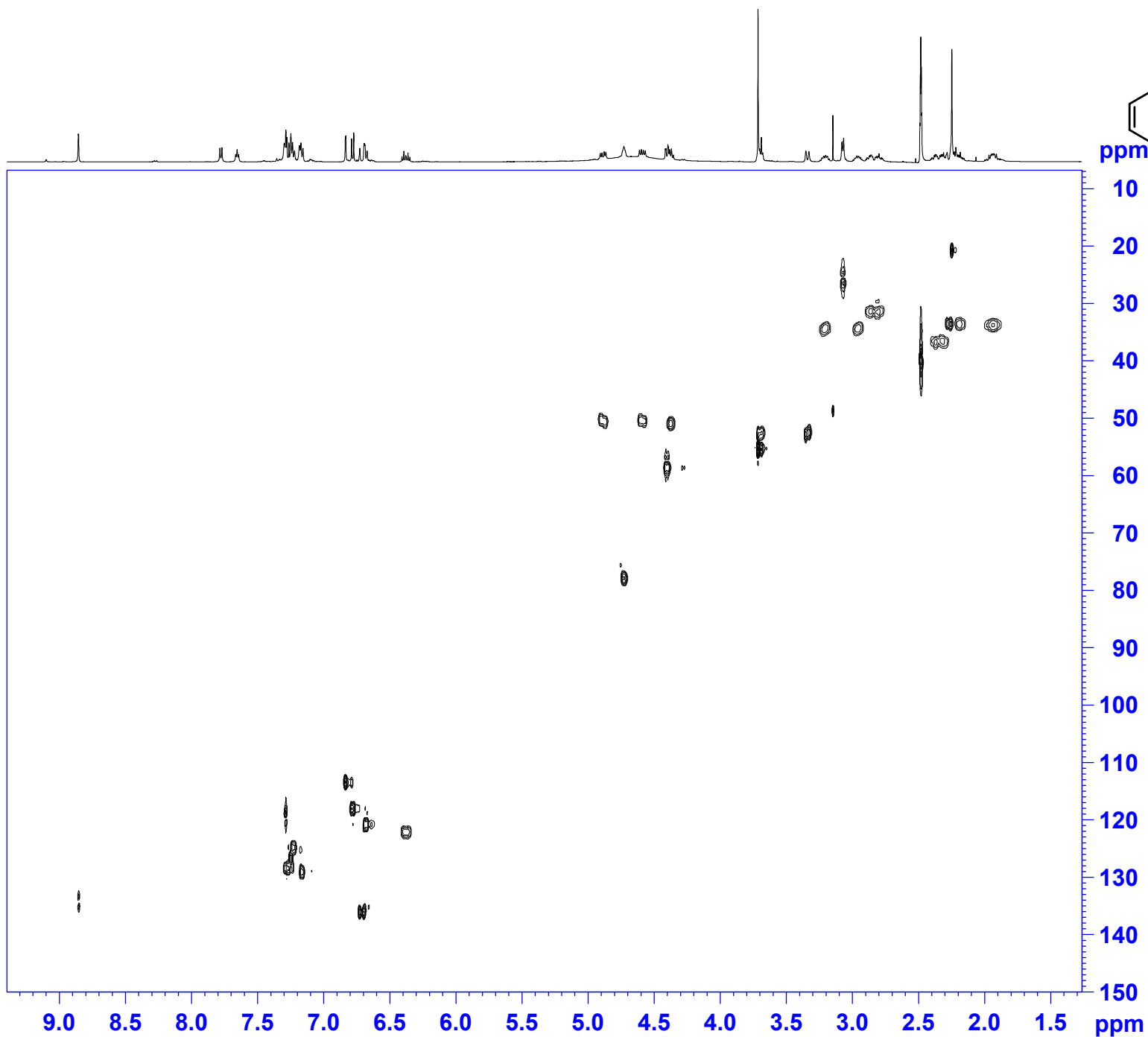




Current Data Parameters
 NAME KL-4-221B_F7
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20120731
 Time_ 19.33
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG cosygmfph
 TD 4096
 SOLVENT DMSO
 NS 2
 DS 8
 SWH 5498.534 H:
 FIDRES 1.342415 H:
 AQ 0.3724629 s:
 RG 44.31
 DW 90.933 u:
 DE 10.00 u:
 TE 296.0 K
 d0 -0.00001273 s:
 D1 2.00000000 s:
 d13 0.00000400 s:
 D16 0.00020000 s:
 DELTA 0.00120400 s:
 in0 0 sec
 ST1CNT 128
 d0orig -0.00001273 s:
 phlloop 0
 t1loop 0
 SFO1 500.1327507 MHz
 NUC1 1H
 P1 10.00 u:
 P2 20.00 u:
 PLW1 13.50000000 W
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPZ1 10.00 %
 GPZ2 20.00 %
 P16 1000.00 u:

F1 - Acquisition parameters:
 TD 256
 SFO1 500.1328 MHz
 FIDRES 19.536423 H:



Current Data Parameters

NAME KL-4-221B_F7
 EXPNO 5
 PROCNO 1

F1 - Acquisition parameters

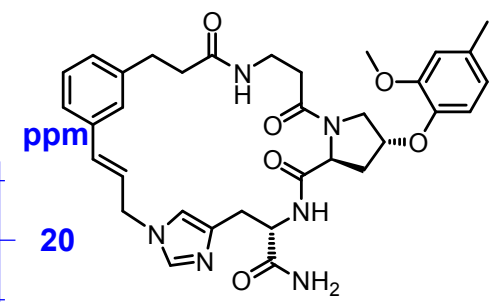
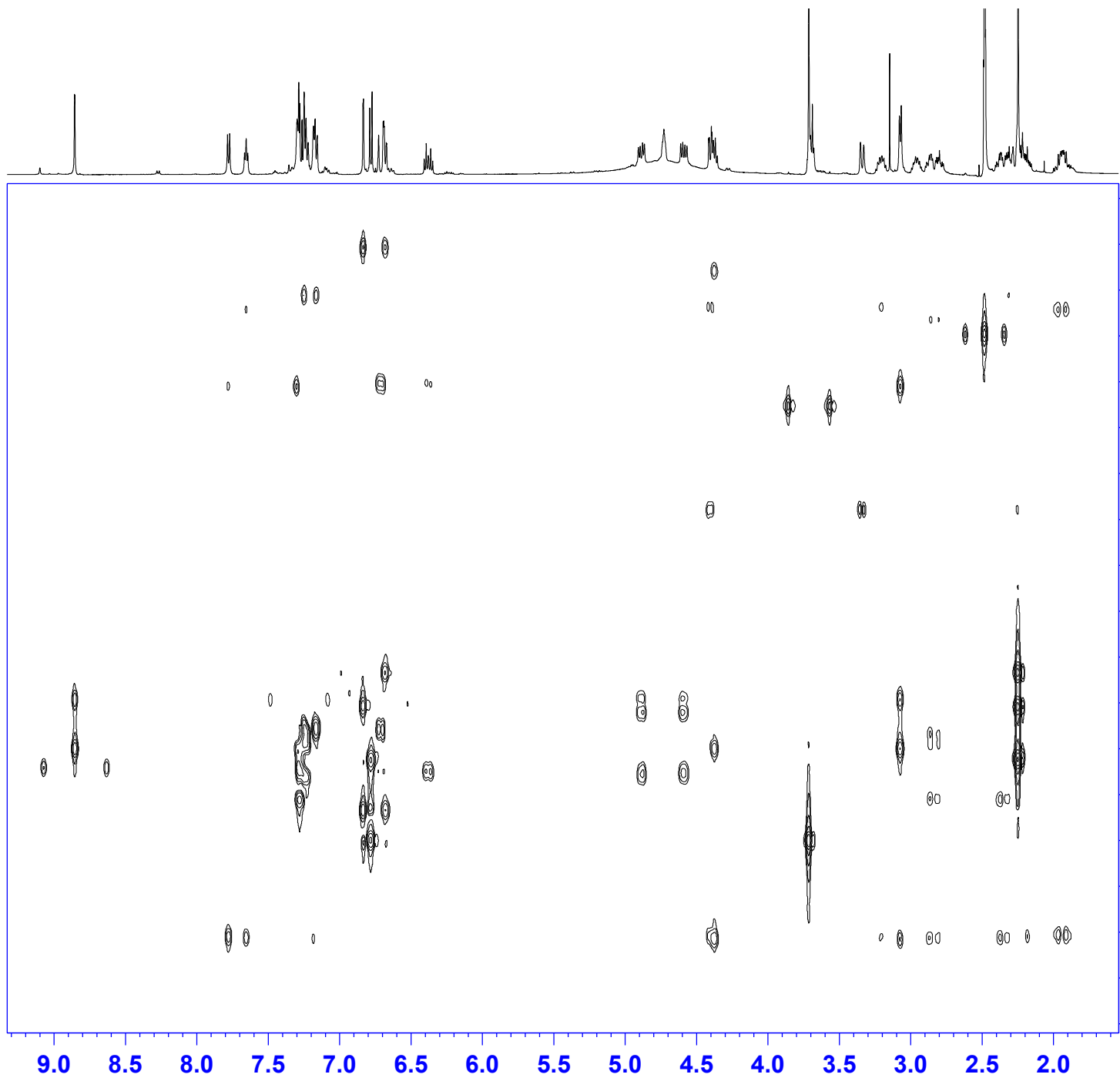
TD 256
 SFO1 125.7678 MHz
 FIDRES 98.255890 Hz
 SW 200.000 ppm
 FnMODE Echo-Antiecho

F2 - Processing parameters

SI 2048
 SF 500.1300135 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters

SI 2048
 MC2 echo-antiecho
 SF 125.7578472 MHz
 WDW TRAP
 SSB 2
 LB 0 Hz
 GB 0



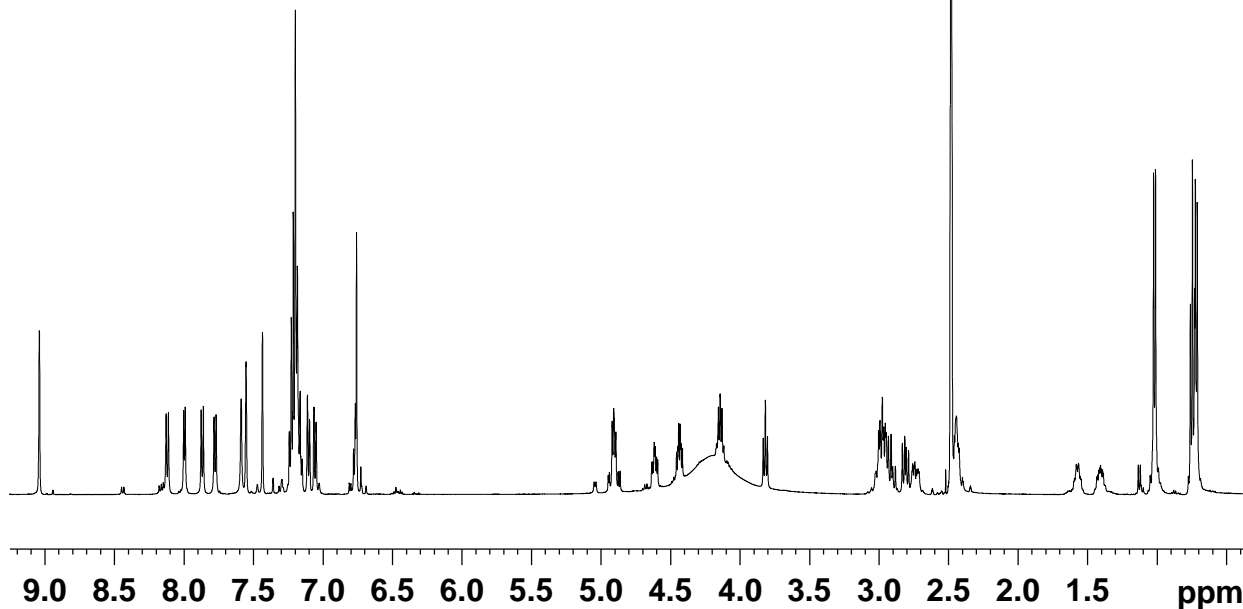
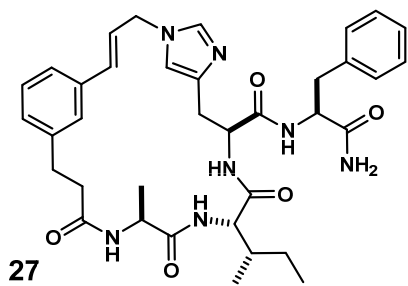
Current Data Parameters
 NAME KL-4-221B_F7
 EXPNO 6
 PROCNO 1

F1 - Acquisition parameters
 TD 120
 SFO1 125.7704 MHz
 FIDRES 209.616226 Hz
 SW 199.999 ppm
 FnmODE QF

F2 - Processing parameters
 SI 2048
 SF 500.1300135 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 QF
 SF 125.7578472 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

Cyclic-Ala-Ile-His-Phe-NH₂ (27):

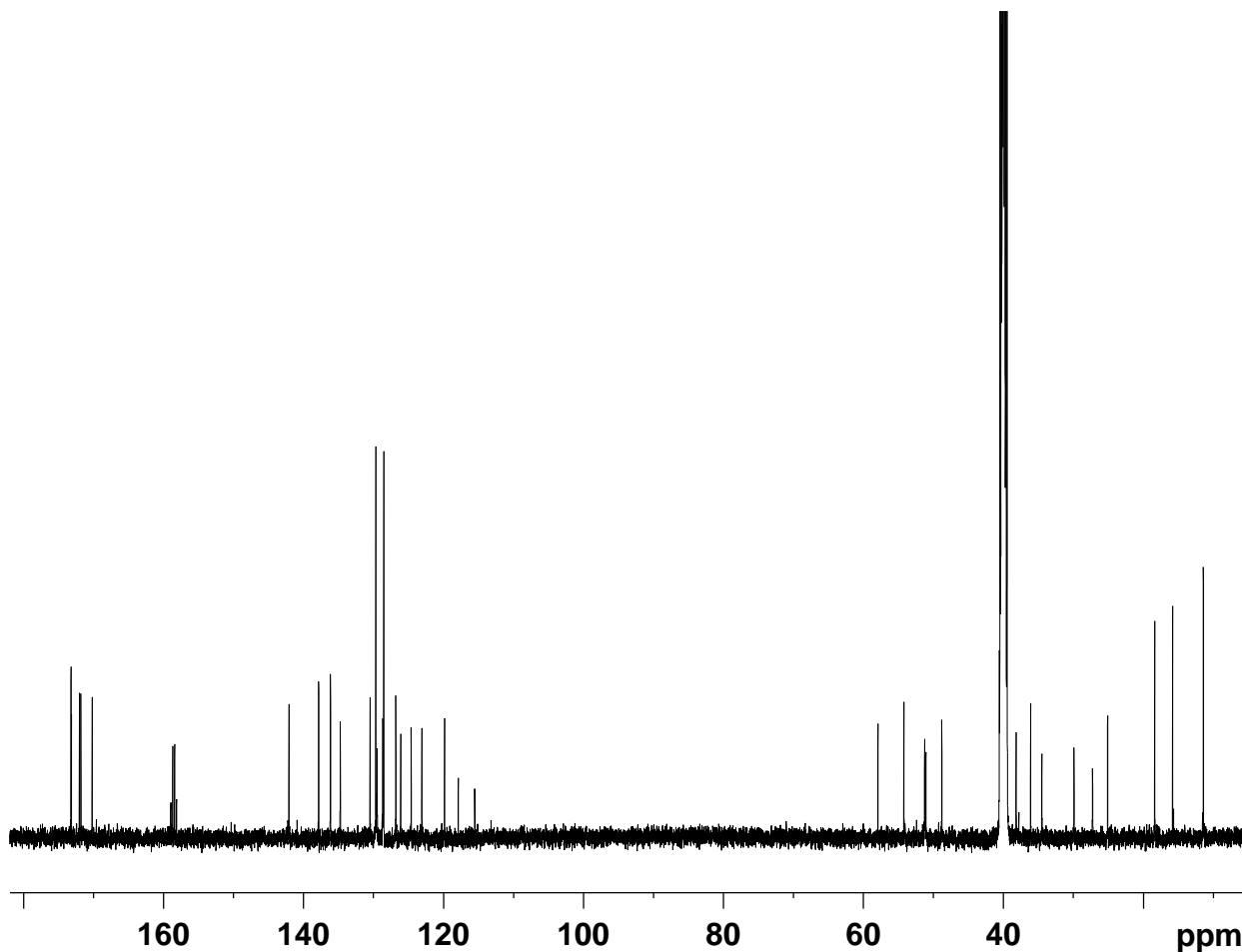


```
Current Data Parameters
NAME      HisA6_cycleF33
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20121208
Time     12.49
INSTRUM  av500
PROBHD   5 mm DCH 13C-1
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       8
DS       0
SWH      10000.000 Hz
FIDRES   0.152588 Hz
AQ       3.2767999 sec
RG       24.37
DW       50.000 usec
DE       10.00 usec
TE       298.0 K
D1       2.0000000 sec
D10      1
TD0      1
```

```
===== CHANNEL f1 =====
SFO1    500.1330008 MHz
NUC1     1H
P1       10.00 usec
PLW1    13.5000000 W
```

```
F2 - Processing parameters
SI       65536
SF       500.1300146 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.40
```



```
Current Data Parameters
NAME      HisA6_cycleF33
EXPNO    2
PROCNO   1

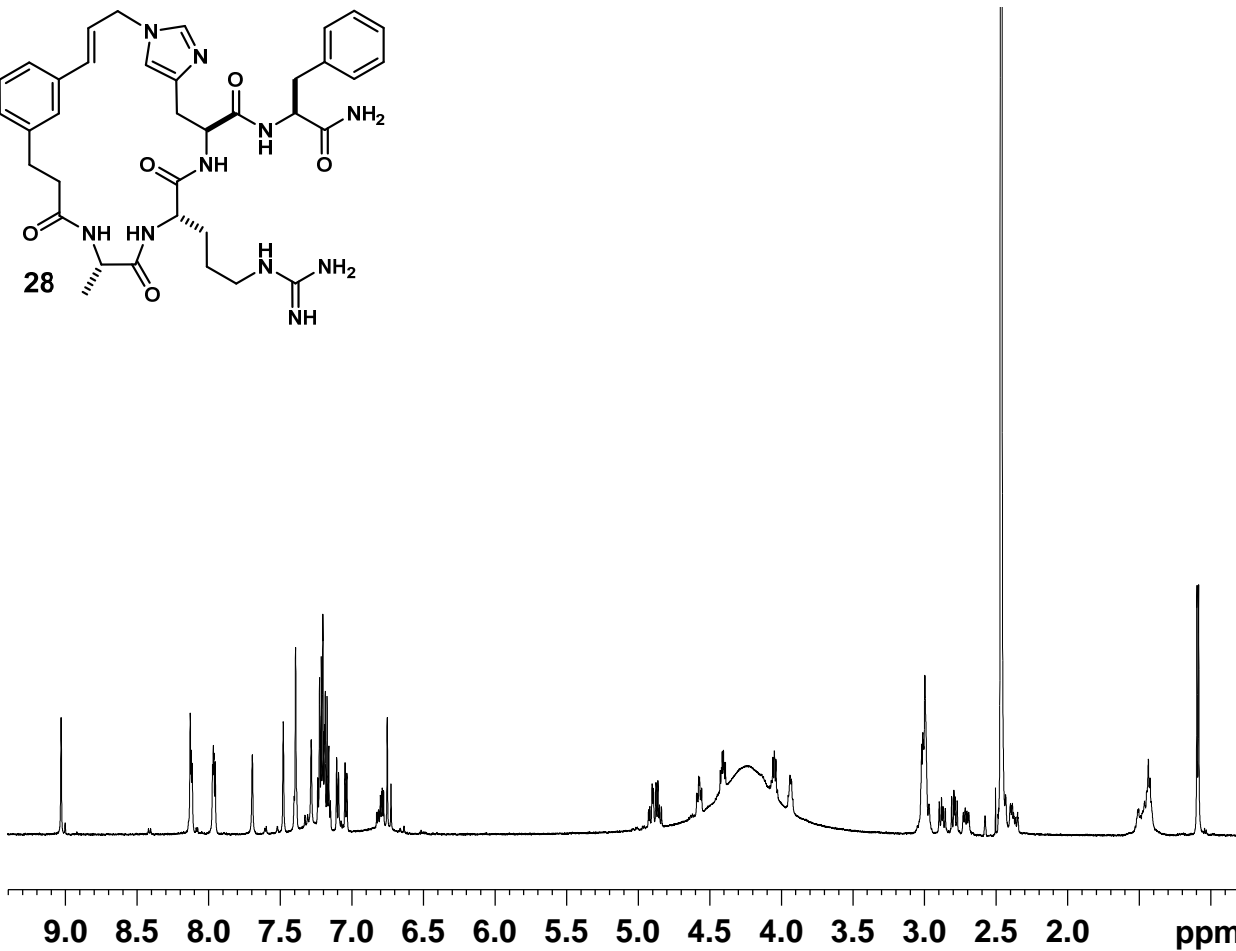
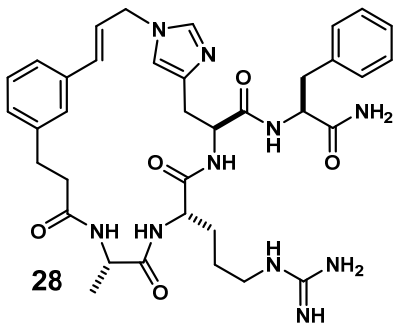
F2 - Acquisition Parameters
Date_    20121208
Time     12.50
INSTRUM  av500
PROBHD   5 mm DCH 13C-1
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       186
DS       2
SWH      31250.000 Hz
FIDRES   0.476837 Hz
AQ       1.0485760 sec
RG       202.91
DW       16.000 usec
DE       18.00 usec
TE       298.0 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
```

```
===== CHANNEL f1 =====
SFO1    125.7722511 MHz
NUC1     13C
P1       9.63 usec
PLW1    23.0000000 W
```

```
===== CHANNEL f2 =====
SFO2    500.1330008 MHz
NUC2     1H
CPDPRG[2] waltz16
PCPD2   80.00 usec
PLW2    13.5000000 W
PLW12   0.21094000 W
PLW13   0.13500001 W
```

```
F2 - Processing parameters
SI       131072
SF       125.7577892 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

Cyclic-Ala-Arg-His-Phe-NH₂ (28):

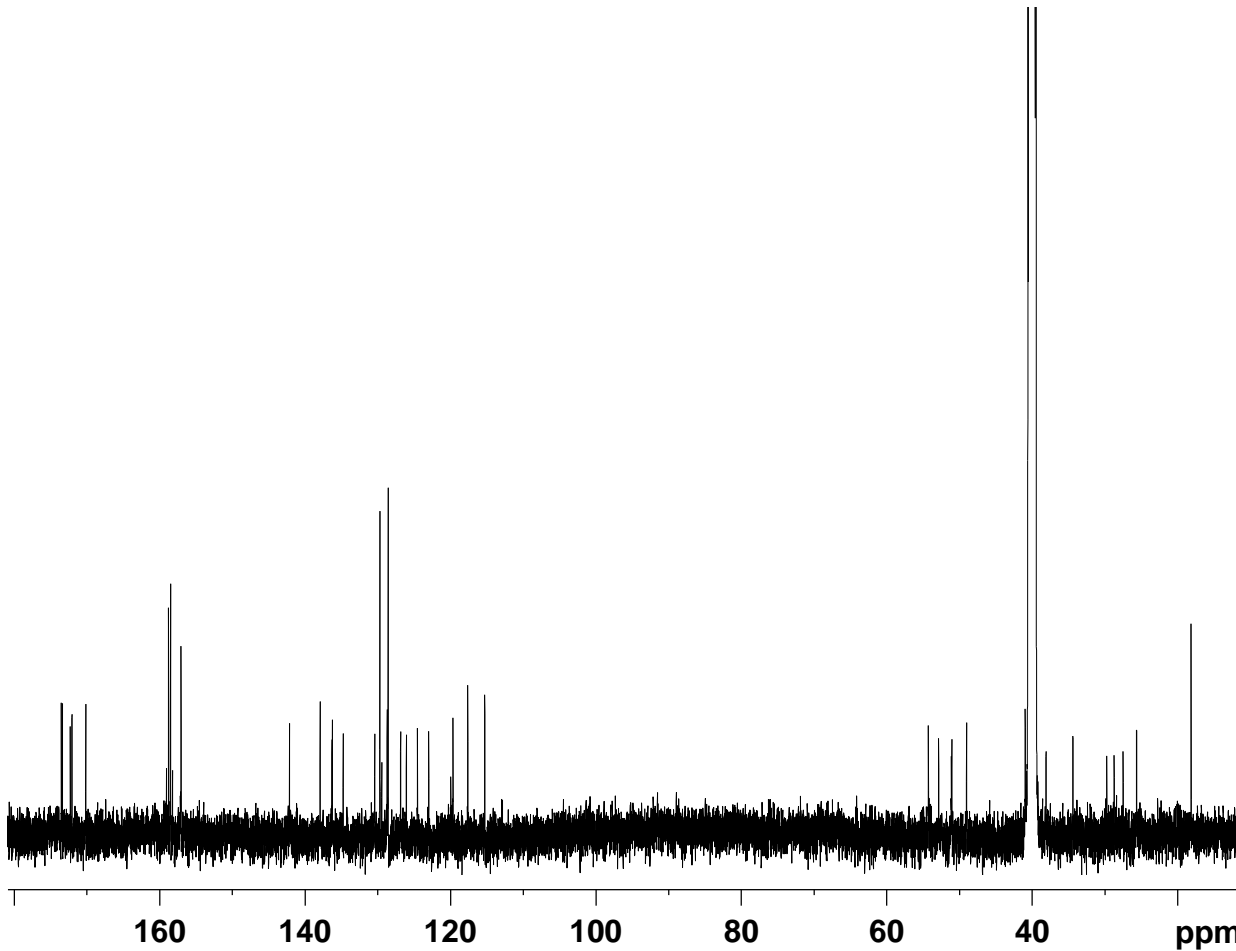


```
Current Data Parameters
NAME His_A5_F24
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121207
Time 17.25
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 12376.237 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 256
DW 40.400 usec
DE 6.50 usec
TE 294.1 K
D1 2.0000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 9.10 usec
PL1 -2.00 dB
PL1W 39.81071854 W
SF01 600.1336008 MHz
```

```
F2 - Processing parameters
SI 65536
SF 600.1300273 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



```
Current Data Parameters
NAME His_A5_F24
EXPNO 2
PROCNO 1

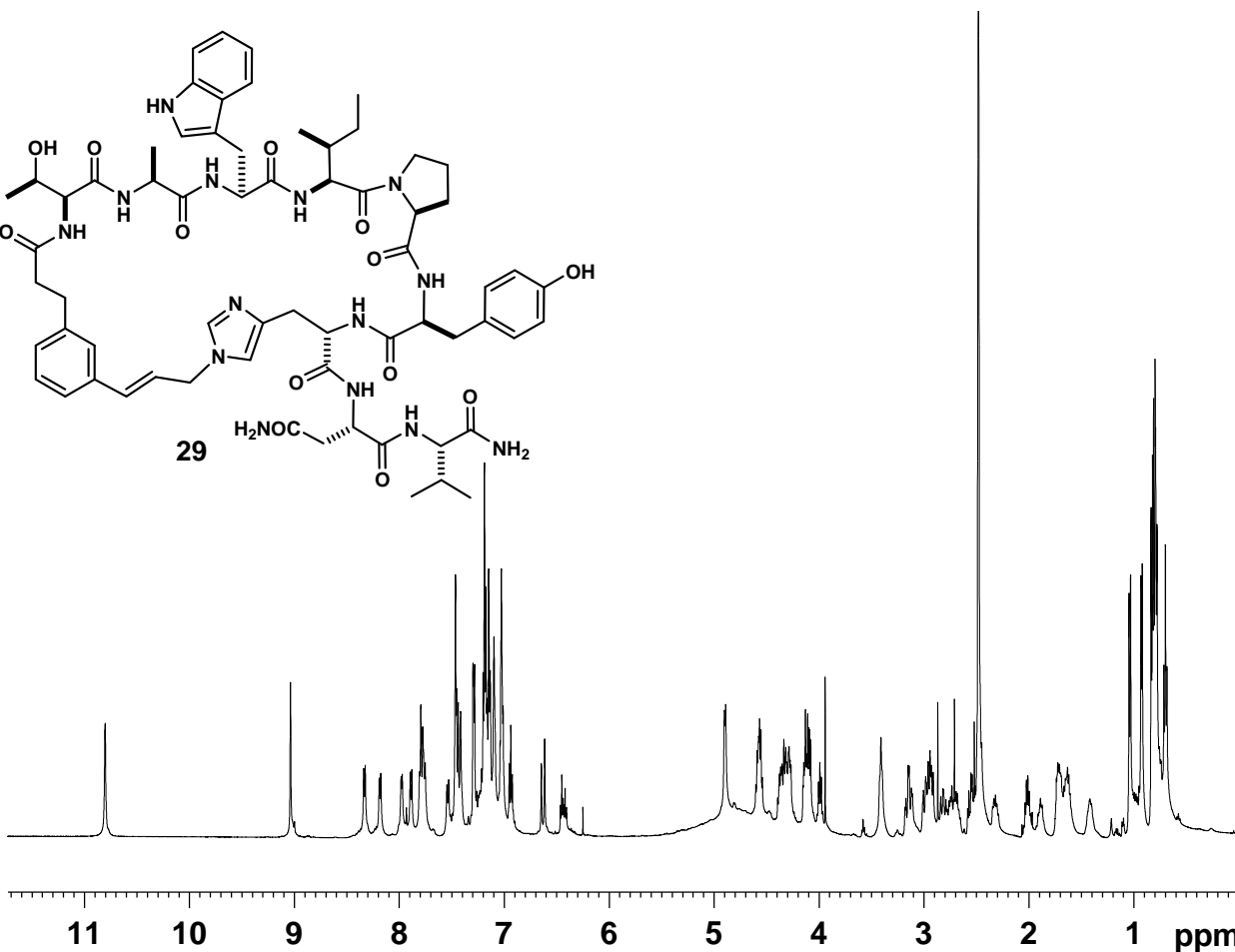
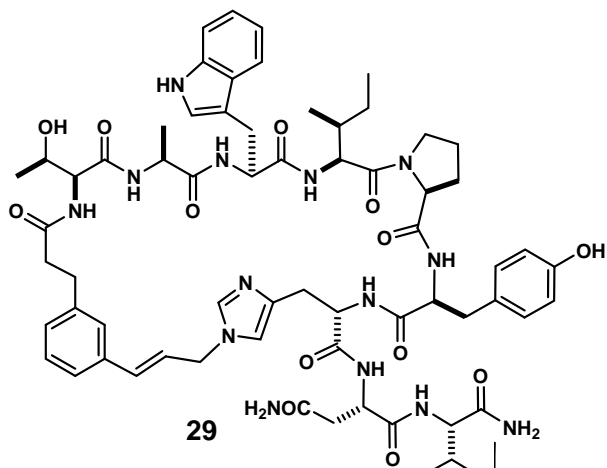
F2 - Acquisition Parameters
Date_ 20130122
Time 10.40
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 472
DS 2
SWH 31250.000 Hz
FIDRES 0.476837 Hz
AQ 1.0485760 sec
RG 202.91
DW 16.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
```

```
===== CHANNEL f1 =====
SF01 125.7722511 MHz
NUC1 13C
P1 9.63 usec
PLW1 23.00000000 W
```

```
===== CHANNEL f2 =====
SF02 500.1330008 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.50000000 W
PLW12 0.21094000 W
PLW13 0.13500001 W
```

```
F2 - Processing parameters
SI 131072
SF 125.7577892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

Cyclic-Thr-Ala-Trp-Ile-Pro-Tyr-His-Asn-Val (29):

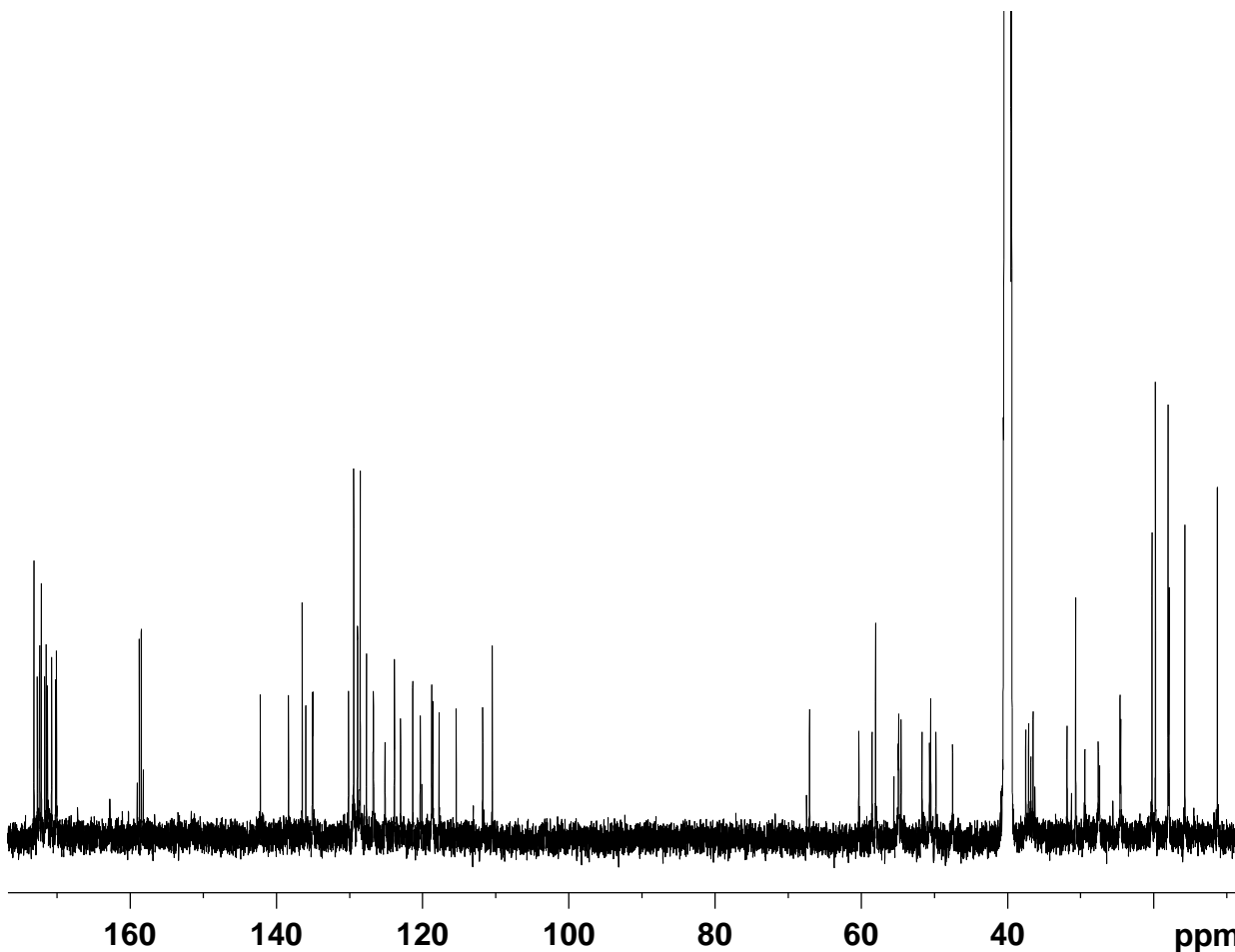


```
Current Data Parameters
NAME      K1-4-184B
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20120419
Time      19.16
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        10000.000 Hz
FIDRES     0.152588 Hz
AQ         3.2767999 sec
RG         160.04
DW         50.000 usec
DE         10.00 usec
TE         296.0 K
D1         2.00000000 sec
D10        1
```

```
===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
PLW1     13.5000000 W
SFO1     500.1330008 MHz
```

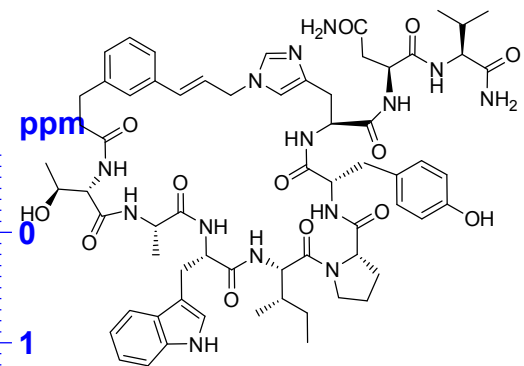
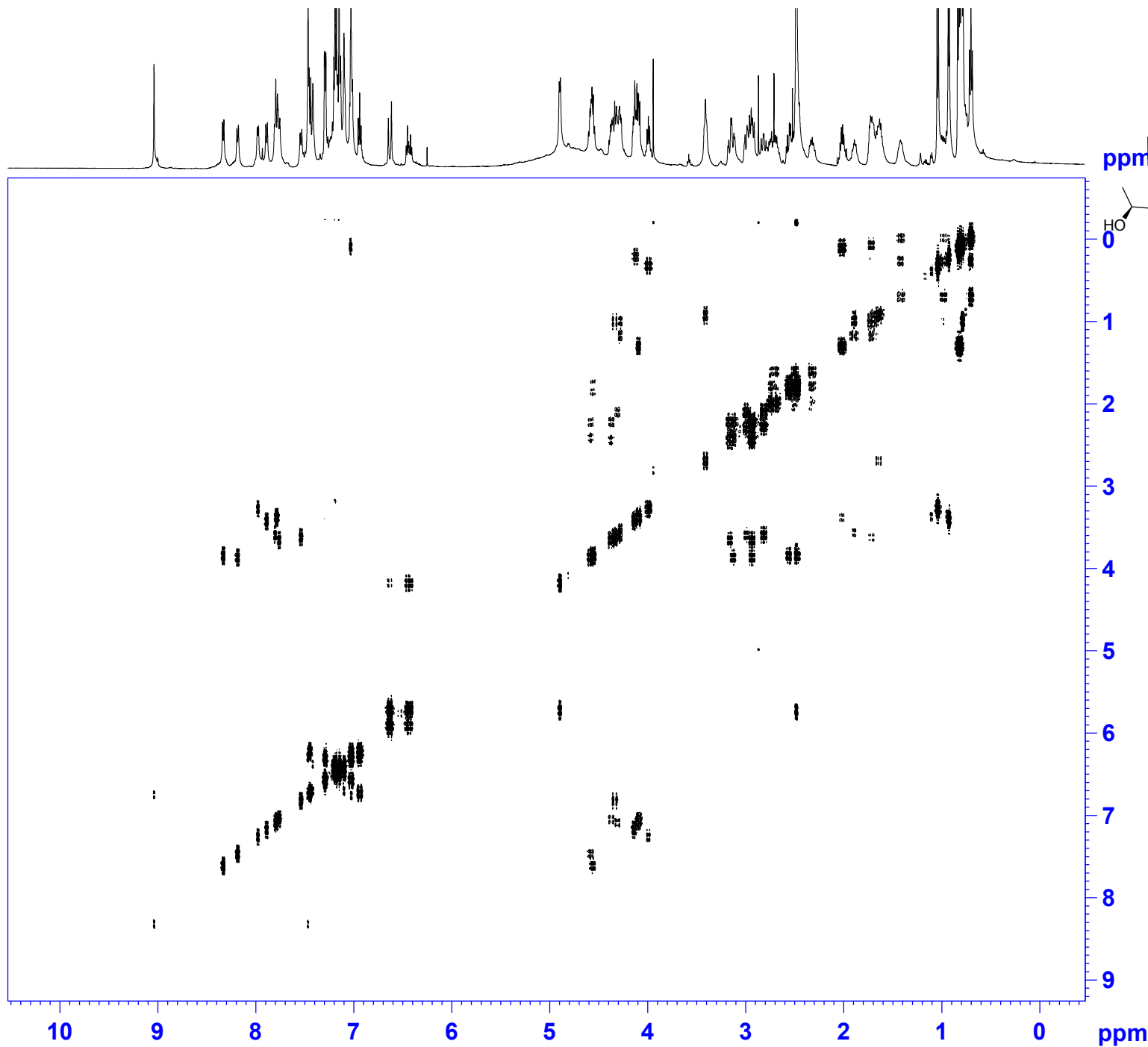
```
F2 - Processing parameters
SI        65536
SF        500.1300146 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```



```
Current Data Parameters
NAME      K1-4-184B
EXPNO     2
PROCNO    1
```

```
F2 - Acquisition Parameters
Date_     20120419
Time      19.18
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         272
DS         2
SWH        31250.000 Hz
FIDRES     0.476837 Hz
AQ         1.0485760 sec
RG         202.91
DW         16.000 usec
DE         18.00 usec
TE         296.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
SFO1     125.7722511 MHz
NUC1      13C
P1         9.63 usec
PLW1     23.0000000 W
SFO2     500.1330008 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     80.00 usec
PLW2     13.5000000 W
PLW12    0.2109400 W
PLW13    0.1350000 W
```

```
F2 - Processing parameters
SI        131072
SF        125.7577892 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

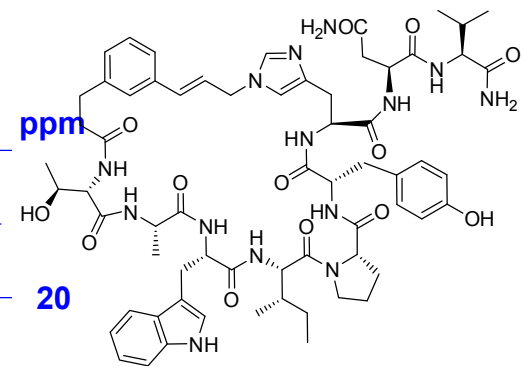
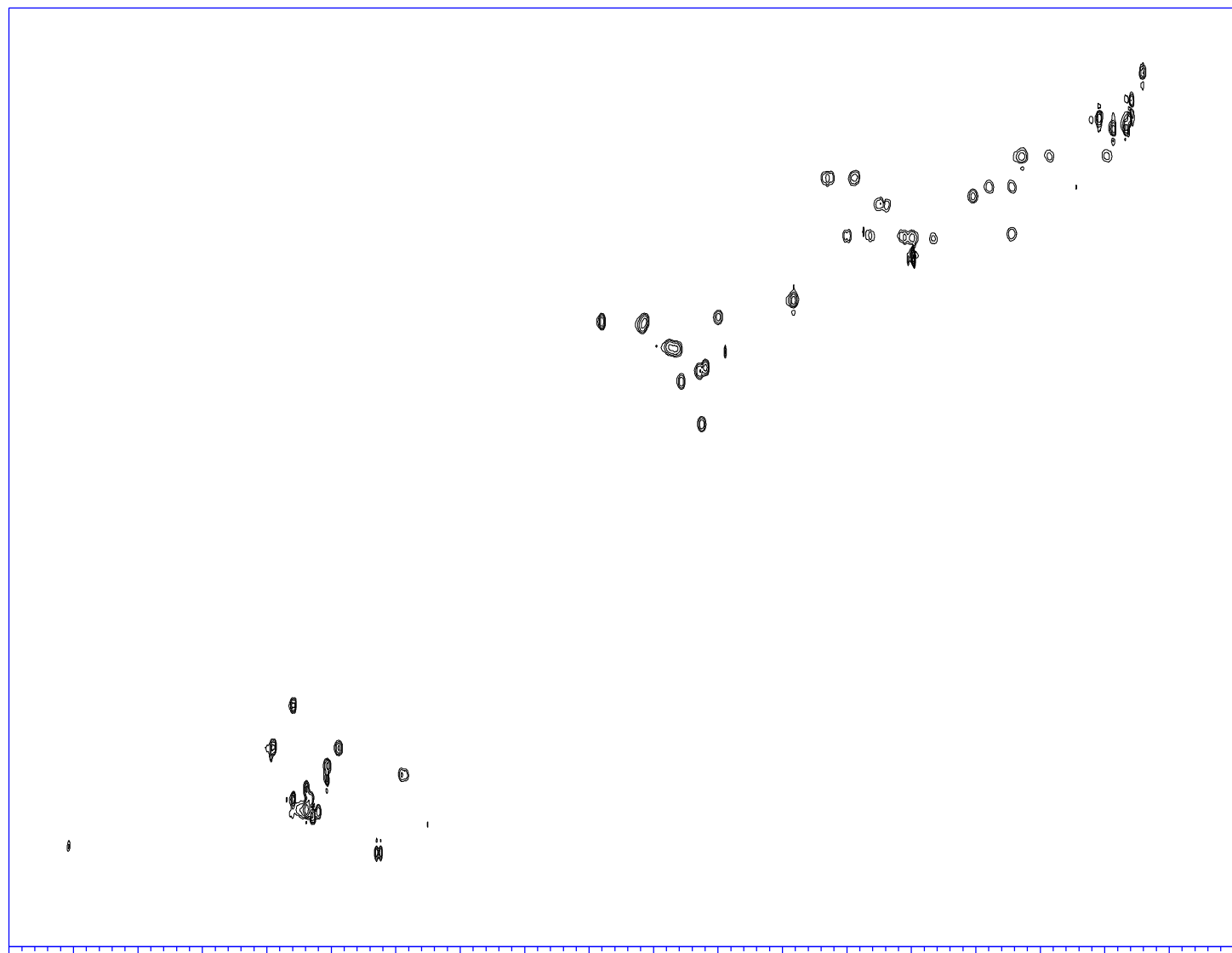
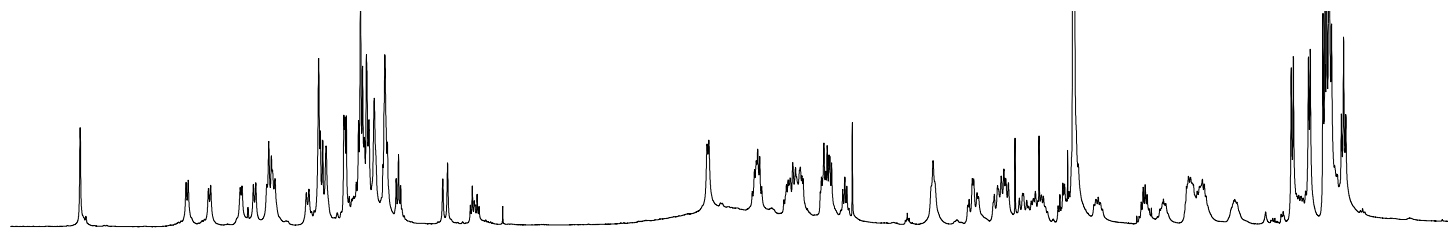


Current Data Parameters
 NAME K1-4-184B
 EXPNO 4
 PROCNO 1

F1 - Acquisition parameters
 TD 256
 SFO1 500.1328 MHz
 FIDRES 19.536423 Hz
 SW 10.000 ppm
 FnmODE States-TPPI

F2 - Processing parameters
 SI 2048
 SF 500.1300135 MHz
 WDW SINE
 SSB 1
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 States-TPPI
 SF 500.1303720 MHz
 WDW SINE
 SSB 1
 LB 0 Hz
 GB 0



Current Data Parameters
 NAME K1-4-184B
 EXPNO 6
 PROCNO 1

F1 - Acquisition parameters
 TD 248
 SFO1 125.7678 MHz
 FIDRES 101.425430 Hz
 SW 200.000 ppm
 FnmODE Echo-Antiecho

F2 - Processing parameters
 SI 2048
 SF 500.1300135 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

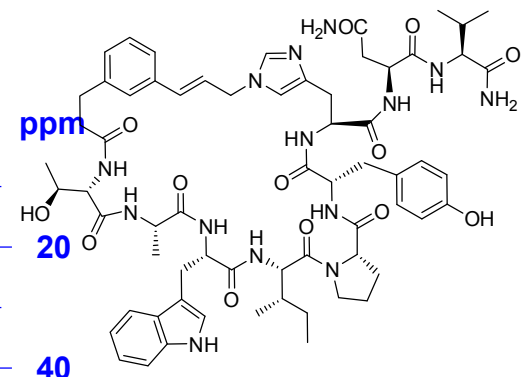
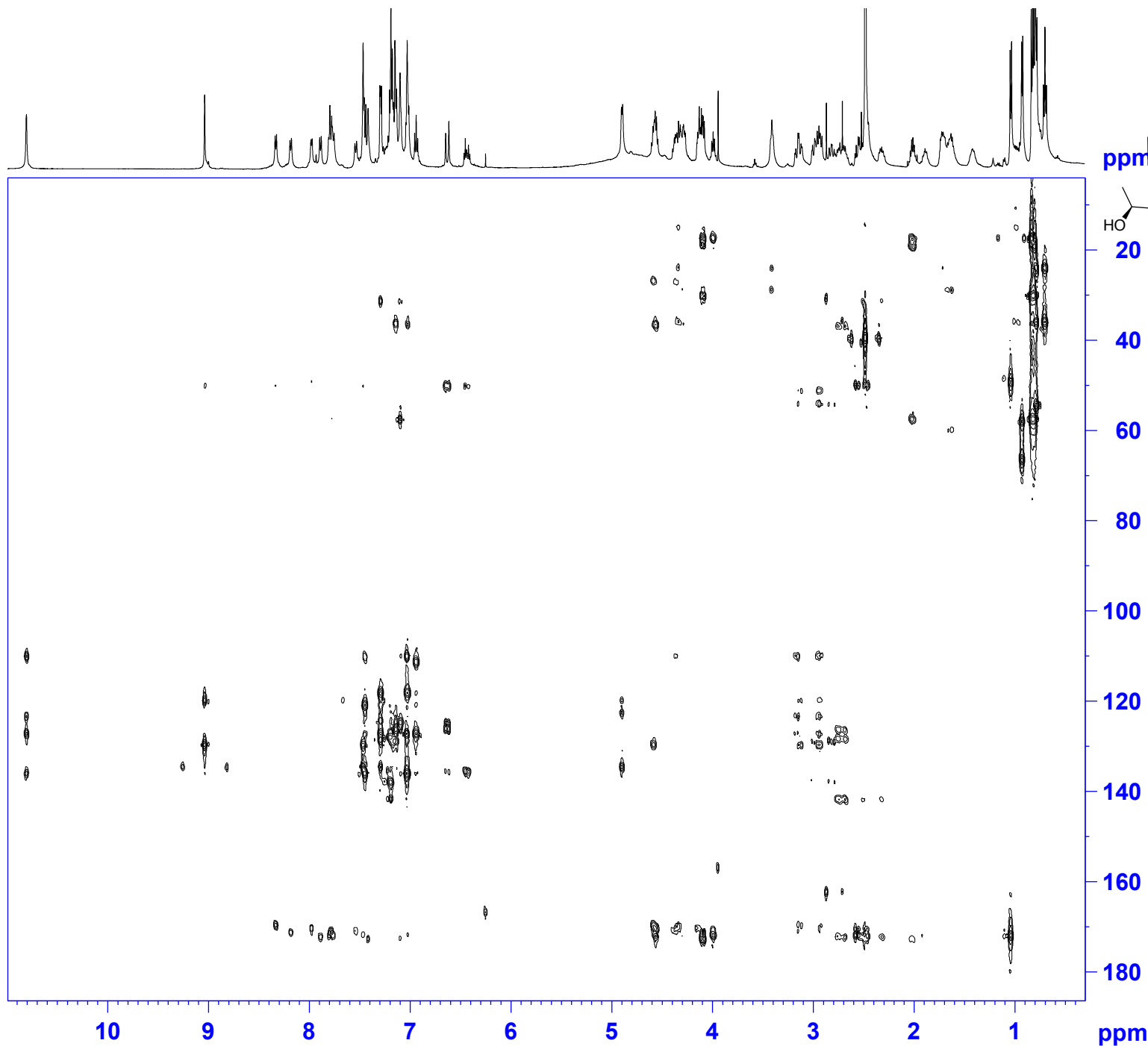
F1 - Processing parameters
 SI 2048
 MC2 echo-antiecho
 SF 125.7578472 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0

100

120

140

ppm



Current Data Parameters

NAME K1-4-184B
 EXPNO 5
 PROCNO 1

F1 - Acquisition parameters

TD 256
 SFO1 125.7704 MHz
 FIDRES 98.257607 Hz
 SW 199.999 ppm
 FnmODE QF

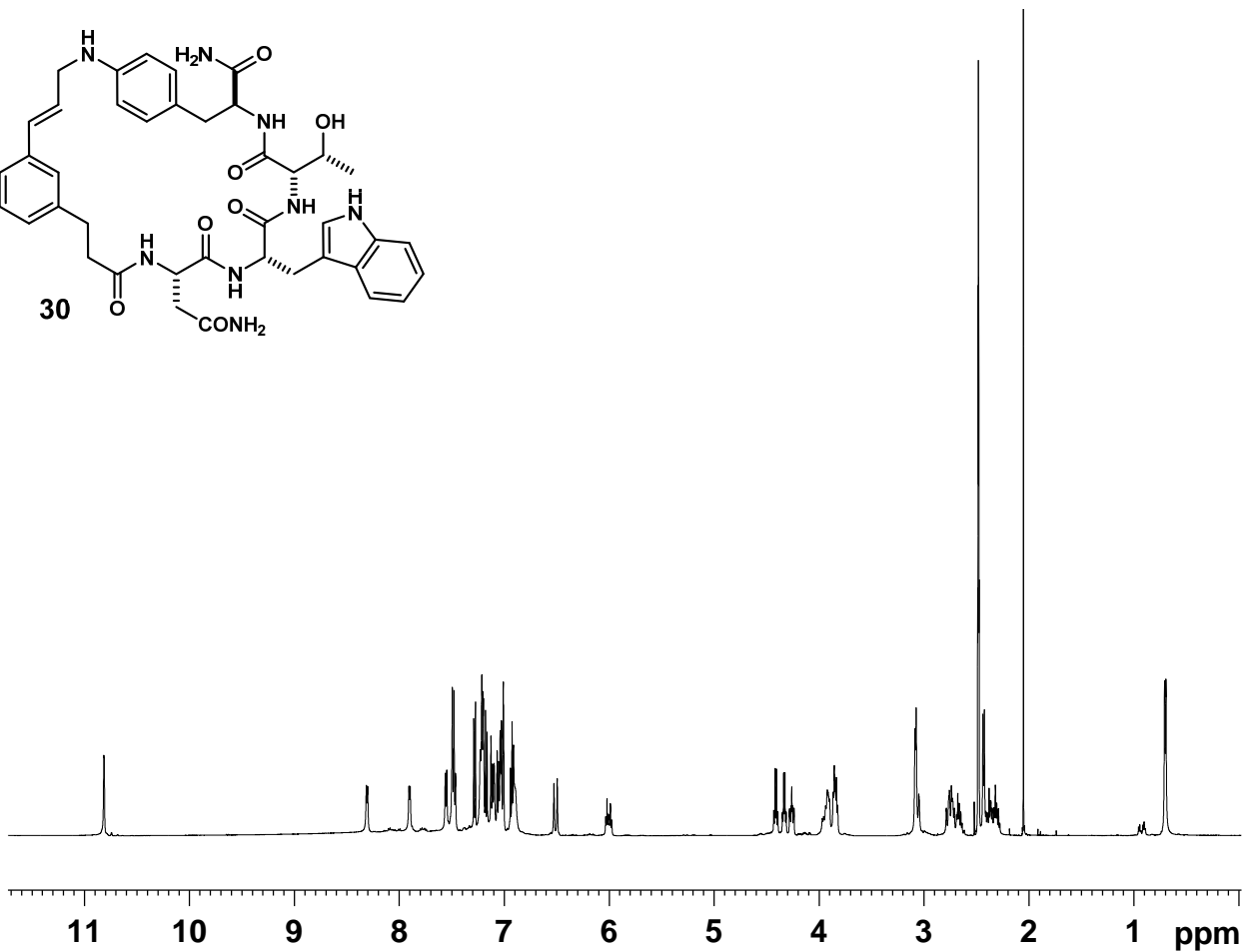
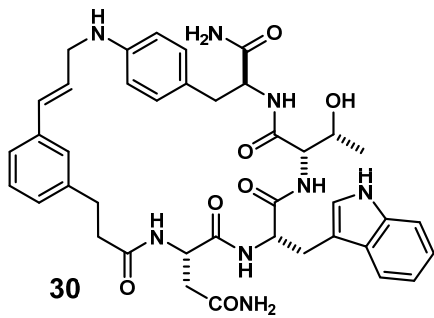
F2 - Processing parameters

SI 2048
 SF 500.1300135 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters

SI 2048
 MC2 QF
 SF 125.7578472 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

Cyclic-Asn-Trp-Thr-Phe(4-NH₂) (30):

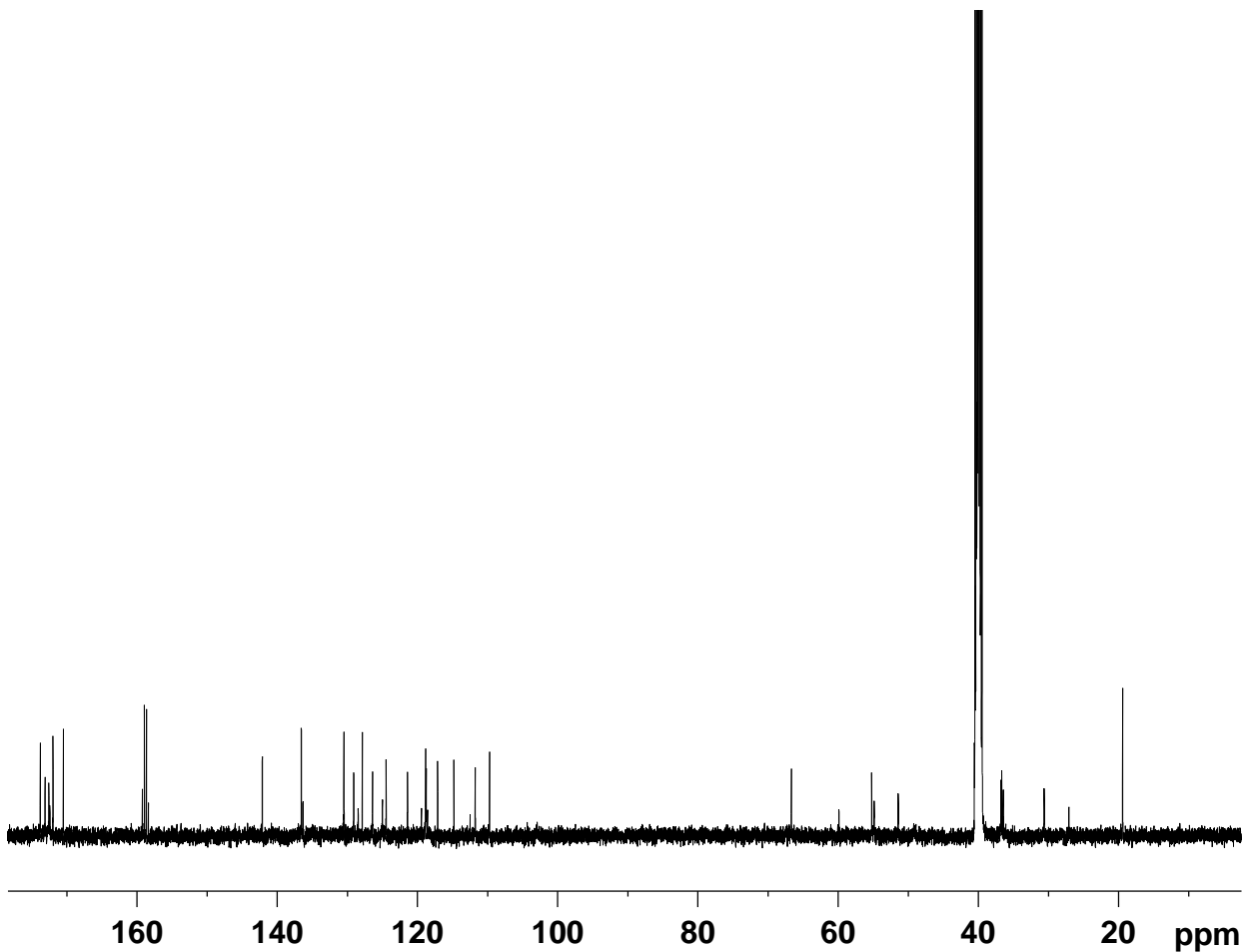


```
Current Data Parameters
NAME          KL-5-158
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20130416
Time          19.41
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            11
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1
```

```
===== CHANNEL f1 =====
SFO1          500.1330008 MHz
NUC1          1H
P1            10.00 usec
PLW1          13.5000000 W
```

```
F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



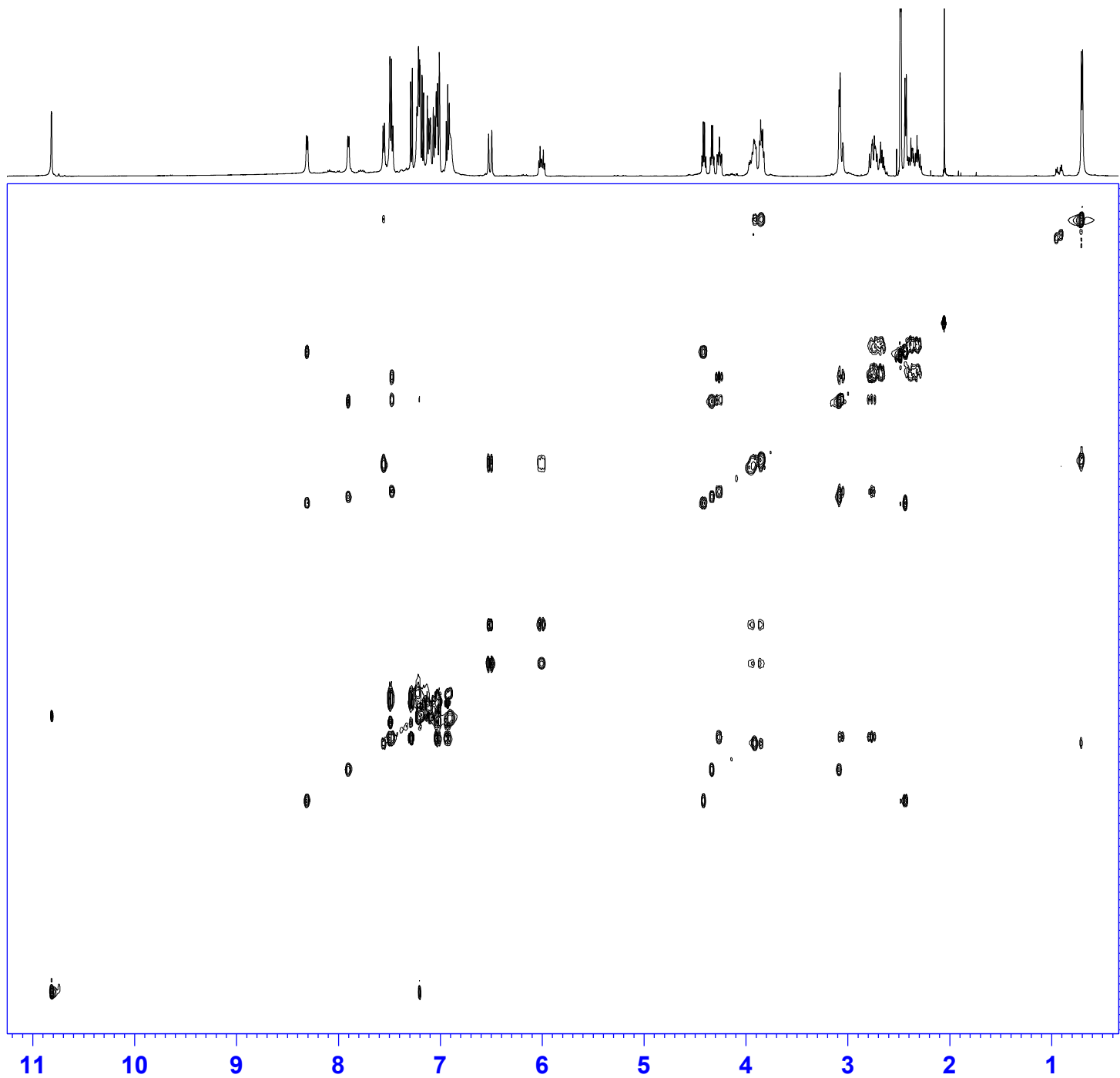
```
Current Data Parameters
NAME          KL-5-158
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20130416
Time          19.45
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            82
DS            2
SWH           31250.000 Hz
FIDRES        0.476837 Hz
AQ            1.0485760 sec
RG            202.91
DW            16.000 usec
DE            18.00 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
```

```
===== CHANNEL f1 =====
SFO1          125.7722511 MHz
NUC1          13C
P1            9.63 usec
PLW1          23.0000000 W
```

```
===== CHANNEL f2 =====
SFO2          500.1330008 MHz
NUC2          1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          13.5000000 W
PLW12         0.21094000 W
PLW13         0.13500001 W
```

```
F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```



ppm

1

2

3

4

5

6

7

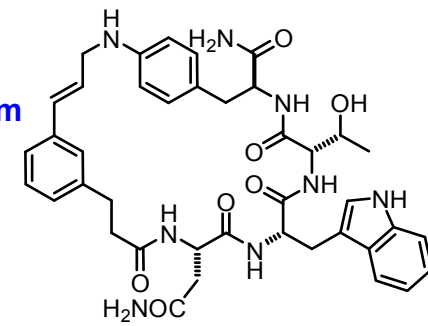
8

9

10

11

ppm

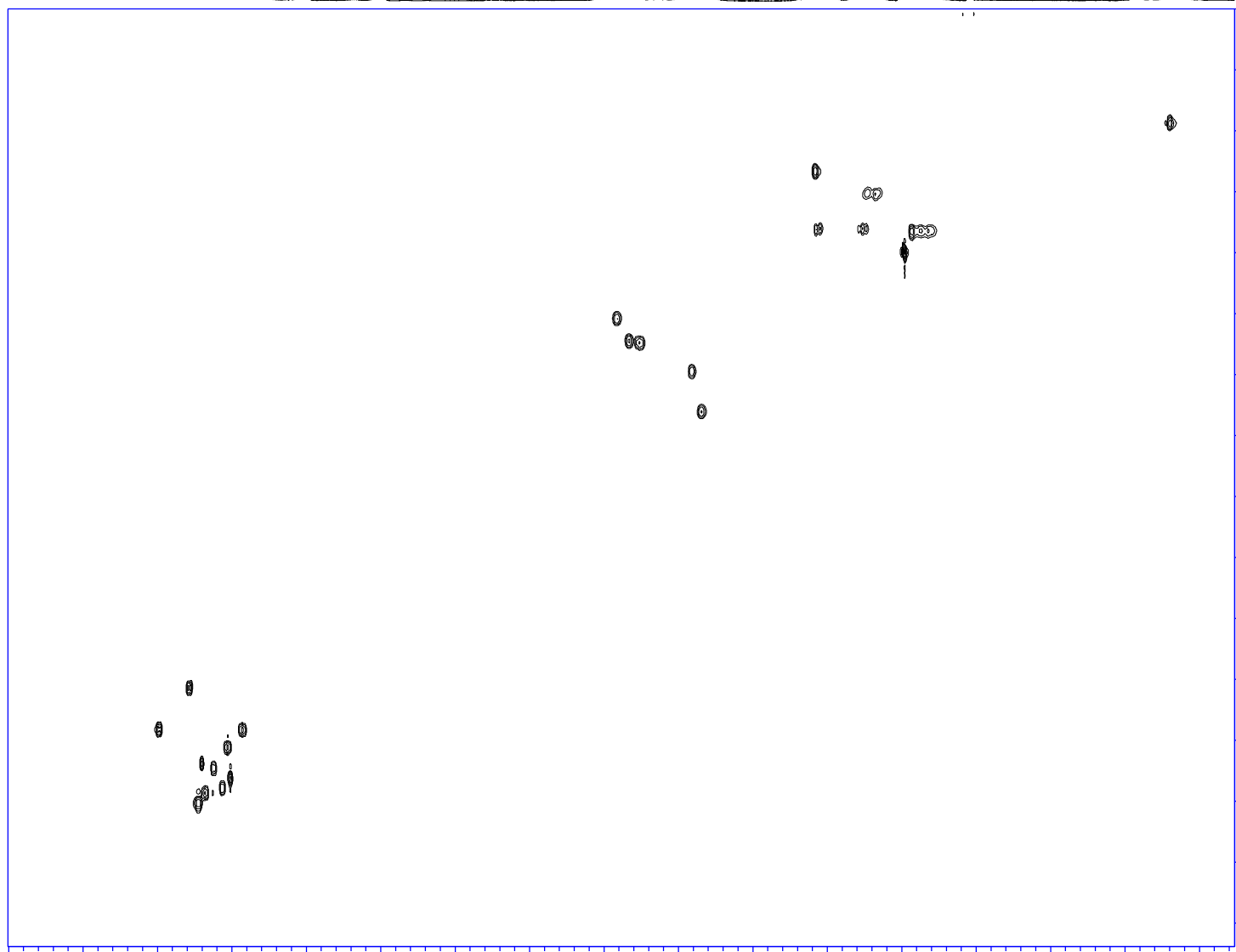
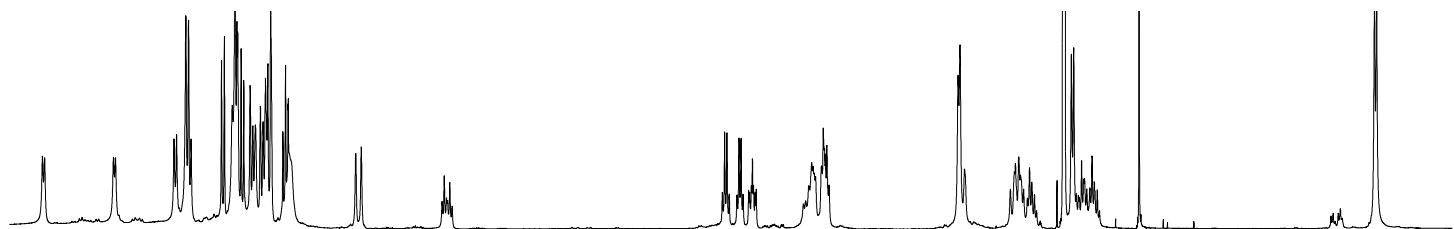


Current Data Parameters
 NAME KL-5-158
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130417
 Time 18.14
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG mlevetgp.js
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 8
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 37.94
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 D0 0.00000300 s:
 D1 2.00000000 s:
 D9 0.06000000 s:
 D11 0.03000000 s:
 D12 0.00002000 s:
 D16 0.00020000 s:
 IN0 0.00016660 s:
 L1 24

===== CHANNEL f1 =====
 SFO1 500.1330008 M:
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 P5 26.68 u:
 P6 40.00 u:
 P7 80.00 u:
 P17 2500.00 u:
 PLW1 13.5000000 W
 PLW10 0.84375000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SINE.100
 GPNAM[2] SINE.100
 GPZ1 30.00 %



ppm

20

40

60

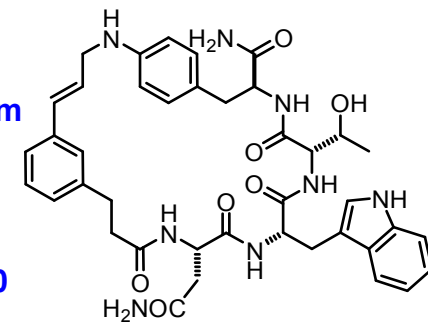
80

100

120

140

ppm

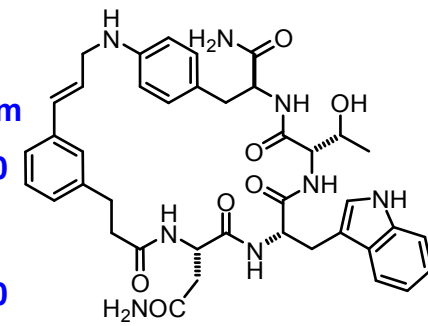
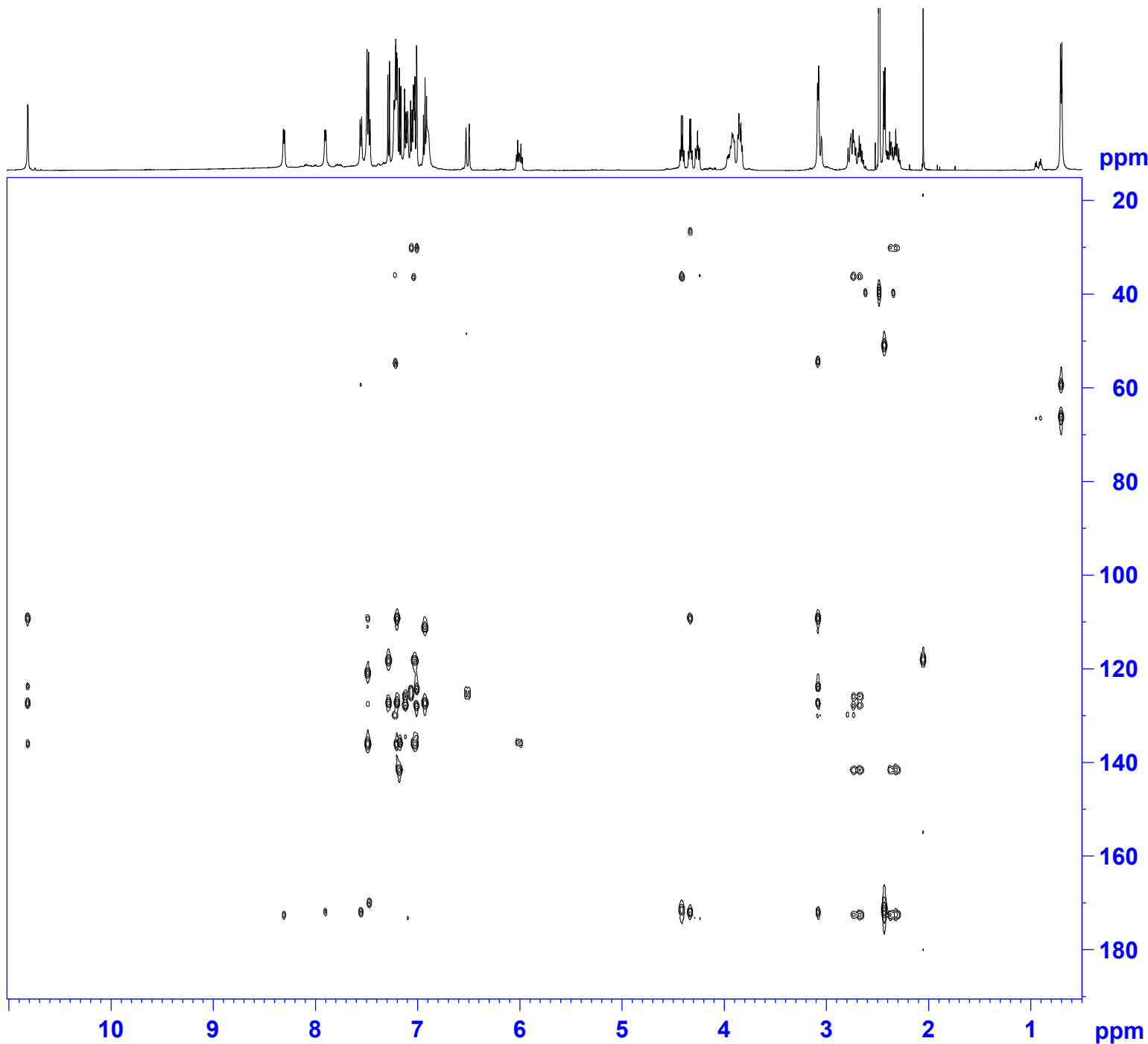


Current Data Parameters
 NAME KL-5-158
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20130417
 Time 18.34
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hsqcedetgp
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 5000.000 H:
 FIDRES 2.441406 H:
 AQ 0.2048000 s:
 RG 202.91
 DW 100.000 u:
 DE 10.00 u:
 TE 298.0 K
 CNST2 145.000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D4 0.00172414 s:
 D11 0.03000000 s:
 D13 0.00000400 s:
 D16 0.00020000 s:
 D21 0.00345000 s:
 IN0 0.00001990 s:
 ZGOPTNS

===== CHANNEL f1 =====
 SFO1 500.1325007 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 P28 0 usec
 PLW1 13.50000000 W

===== CHANNEL f2 =====
 SFO2 125.7678496 MHz
 NUC2 13C
 CPDPRG[2] garp
 P3 9.63 u:
 P4 19.26 u:



Current Data Parameters
 NAME KL-5-158
 EXPNO 7
 PROCNO 1

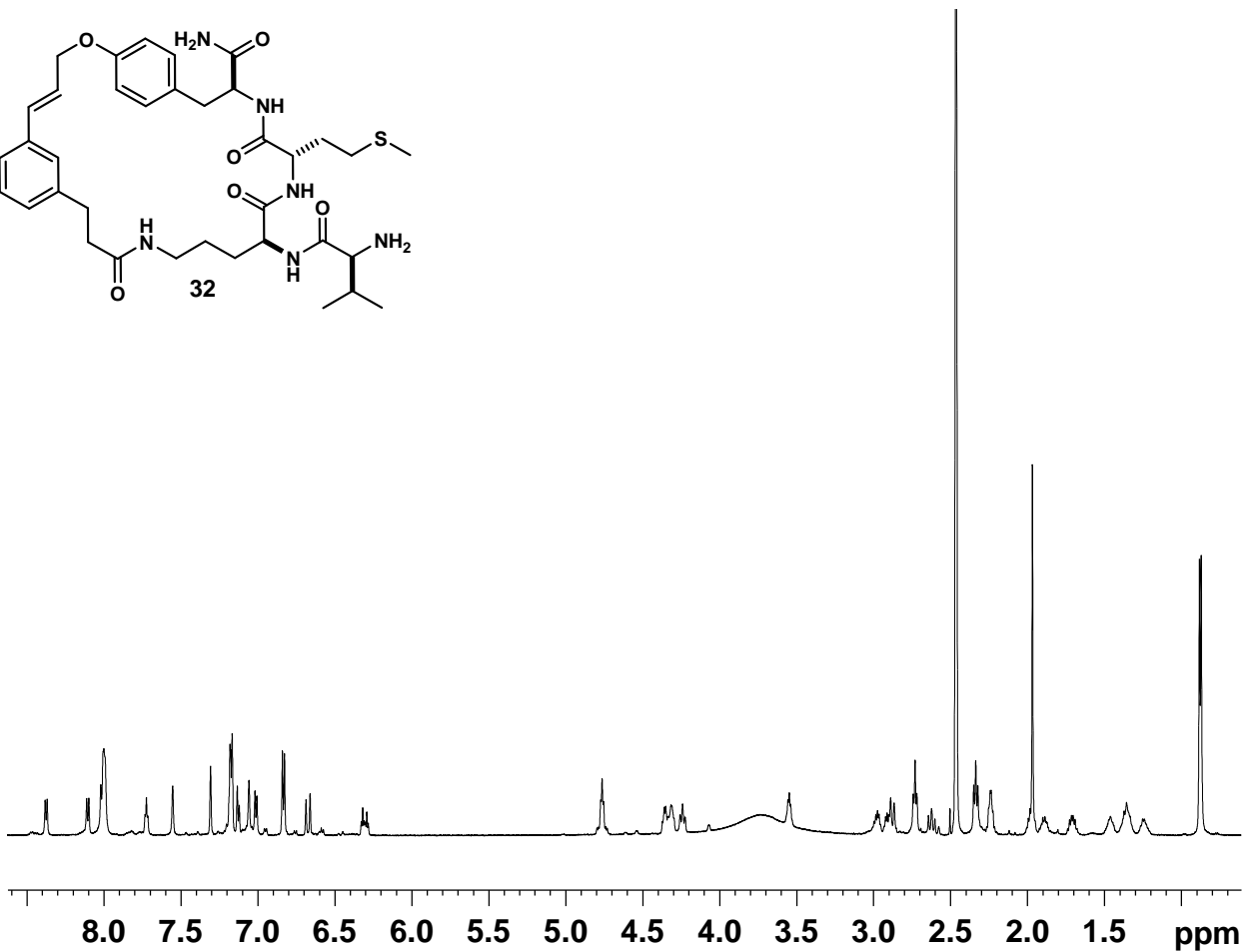
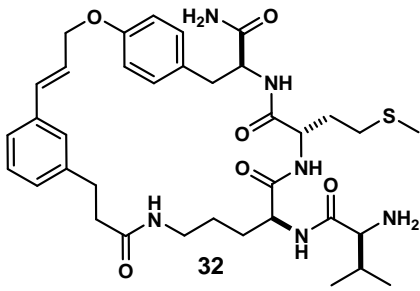
F2 - Acquisition Parameters
 Date_ 20130417
 Time 18.50
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 202.91
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D6 0.07142857 s:
 D16 0.00020000 s:
 IN0 0.00001990 s:

==== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 PLW1 13.50000000 W

==== CHANNEL f2 =====
 SFO2 125.7703648 MHz
 NUC2 13C
 P3 9.63 u:
 PLW2 23.01399994 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100

Cyclic-Val-Orn-Met-Try (32):



```

Current Data Parameters
NAME      KL-5-156C_AV600
EXPNO     1
PROCNO    1

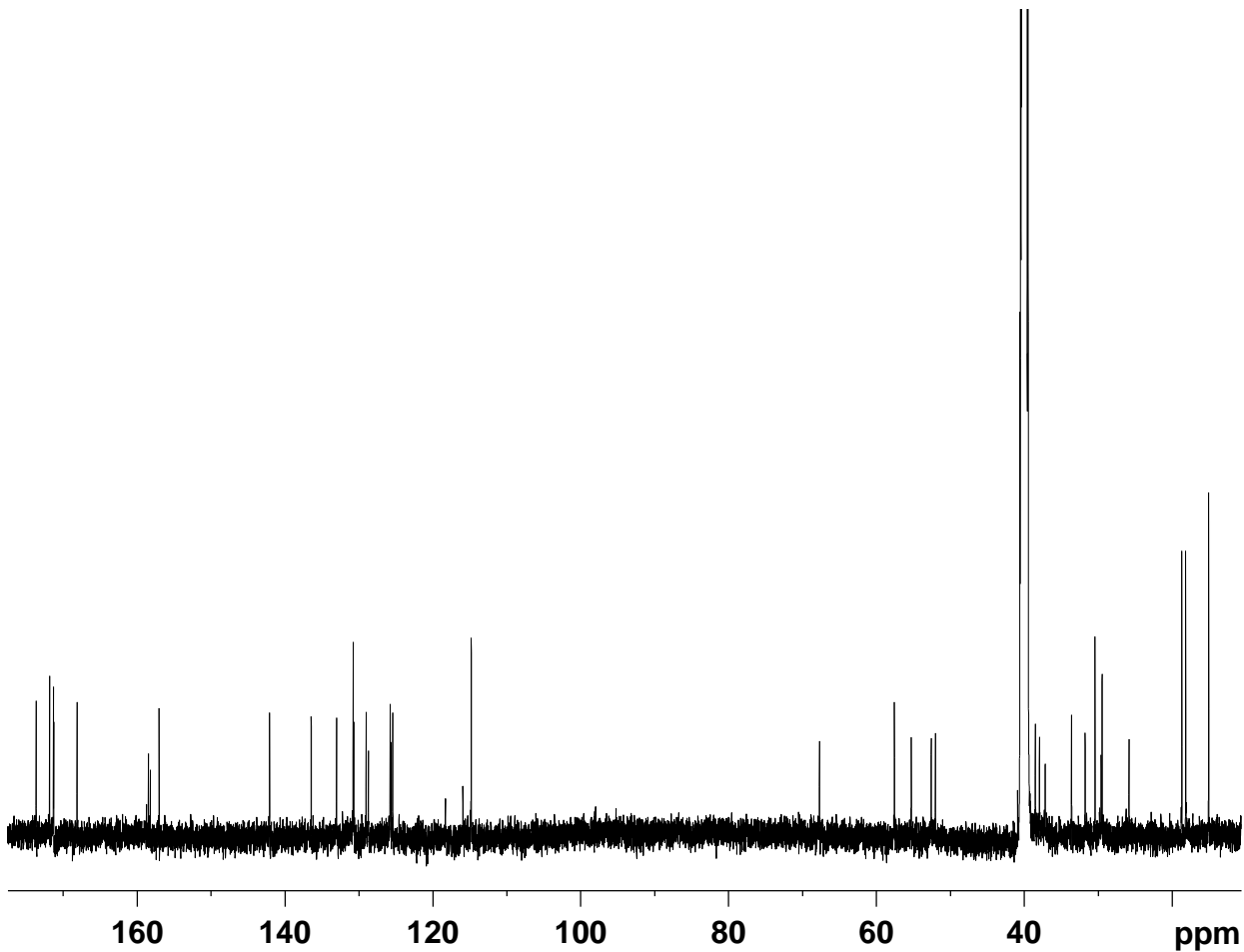
F2 - Acquisition Parameters
Date_     20130411
Time      20.12
INSTRUM   av600
PROBHD    5 mm TBI5
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         8
DS         0
SWH        12376.237 Hz
FIDRES     0.188846 Hz
AQ         2.6476543 sec
RG         181
DW         40.400 usec
DE         6.50 usec
TE         294.1 K
D1         2.00000000 sec
D10        1
    
```

```

===== CHANNEL f1 =====
NUC1       1H
P1         9.75 usec
PL1        -2.00 dB
PL1W       39.81071854 W
SFO1       600.1336008 MHz
    
```

```

F2 - Processing parameters
SI          65536
SF          600.1300273 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.40
    
```



```

Current Data Parameters
NAME      KL-5-156C
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20130425
Time      19.49
INSTRUM   av500
PROBHD    5 mm DCH 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         487
DS         2
SWH        31250.000 Hz
FIDRES     0.476837 Hz
AQ         1.0485760 sec
RG         202.91
DW         16.000 usec
DE         18.00 usec
TE         298.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D10        1
    
```

```

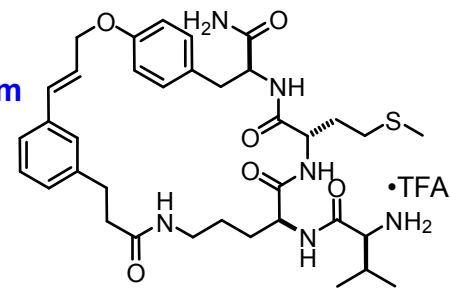
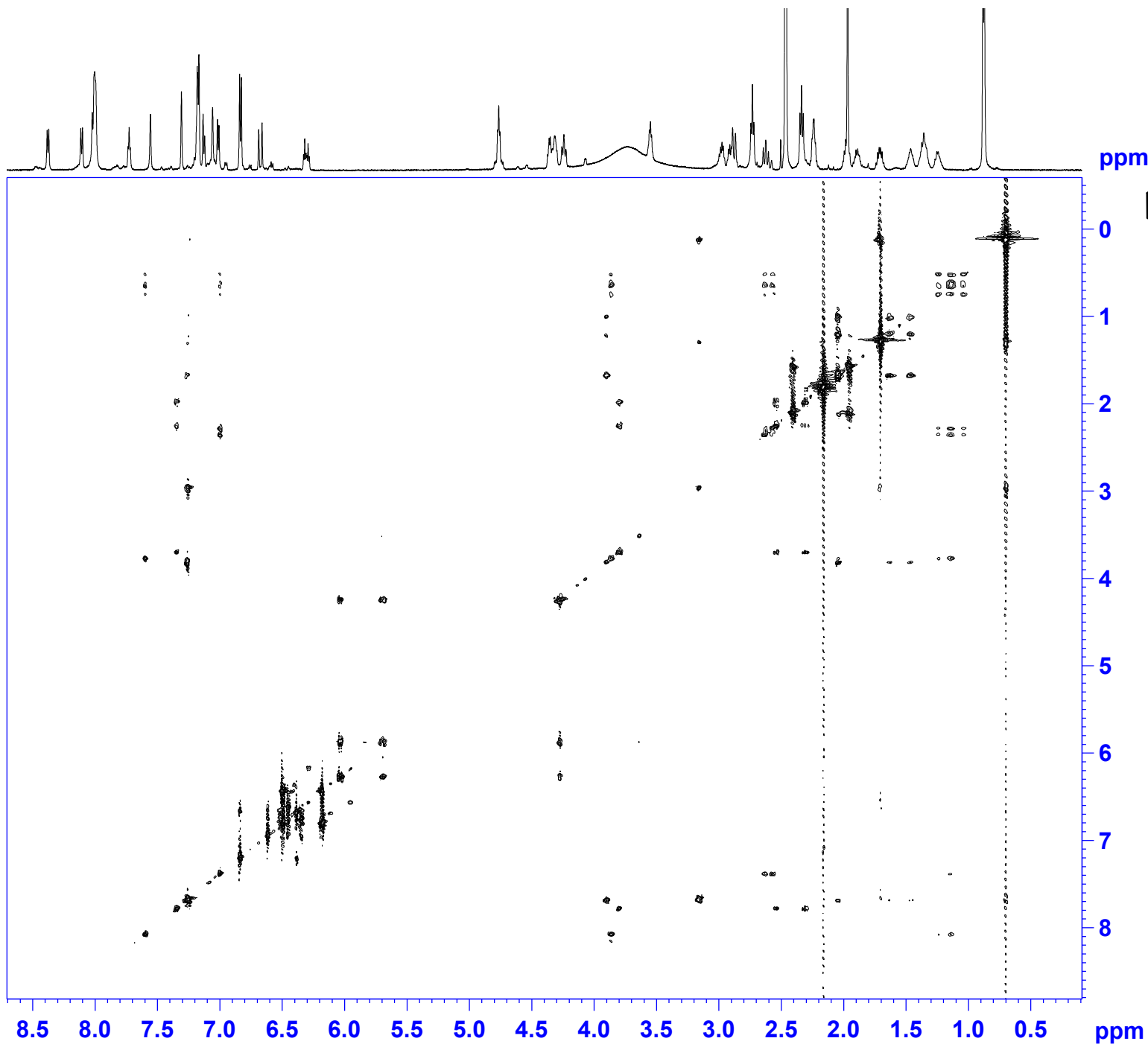
===== CHANNEL f1 =====
SFO1       125.7722511 MHz
NUC1       13C
P1         9.63 usec
PLW1       23.00000000 W
    
```

```

===== CHANNEL f2 =====
SFO2       500.1330008 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2      80.00 usec
PLW2       13.50000000 W
PLW12      0.21094000 W
PLW13      0.13500001 W
    
```

```

F2 - Processing parameters
SI          131072
SF          125.7577892 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

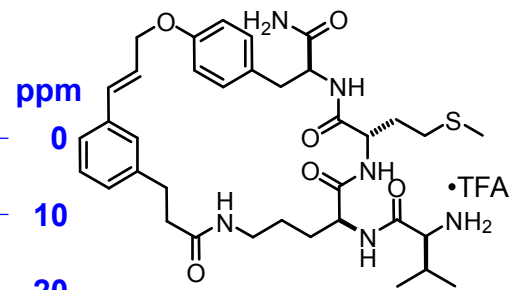
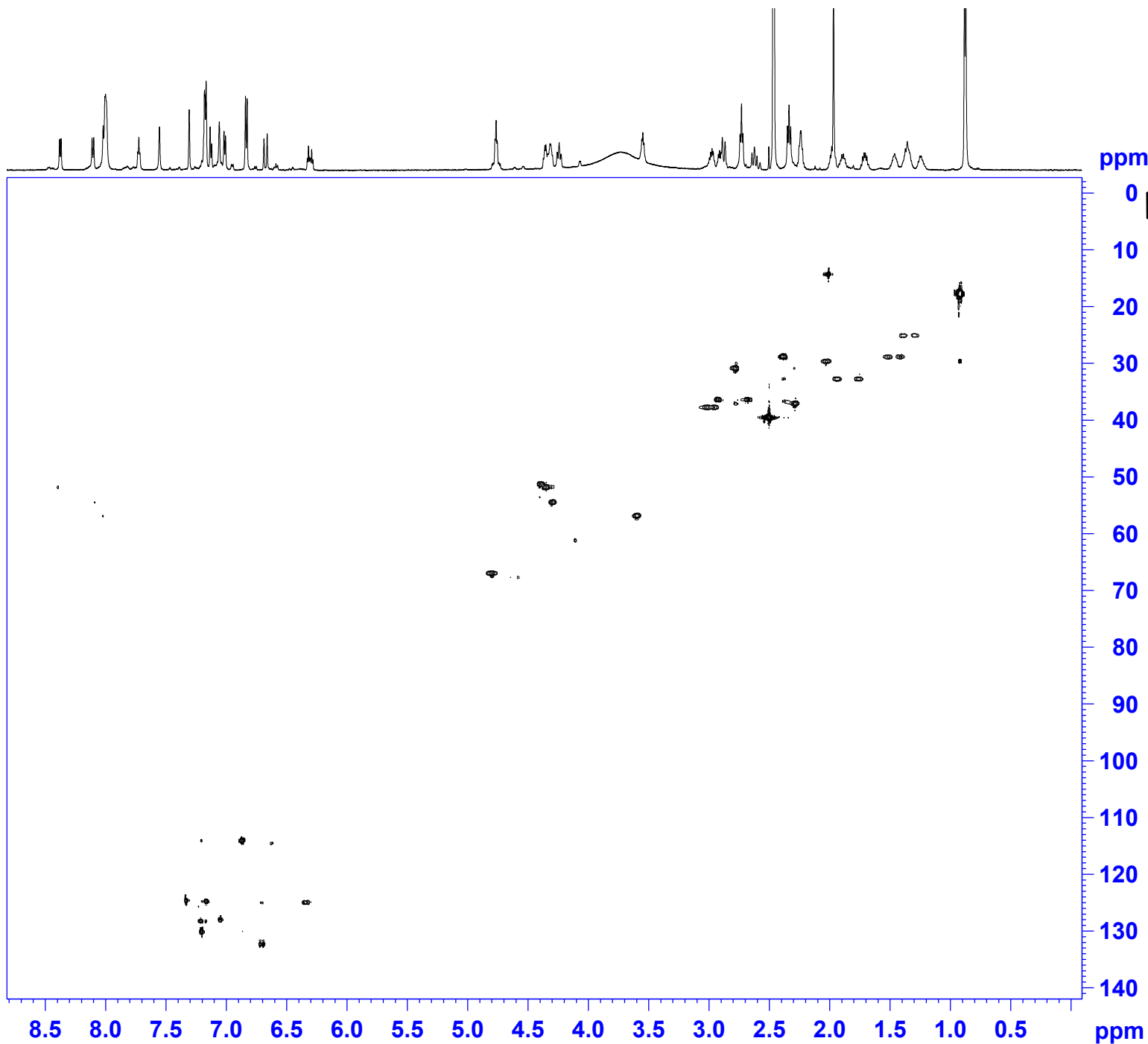


Current Data Parameters
 NAME KL-5-156C_AV600
 EXPNO 3
 PROCNO 1

F1 - Acquisition parameters
 TD 600
 SFO1 600.133 MHz
 FIDRES 10.002216 Hz
 SW 10.000 ppm
 FnMODE Echo-Antiecho

F2 - Processing parameters
 SI 1024
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 echo-antiecho
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0

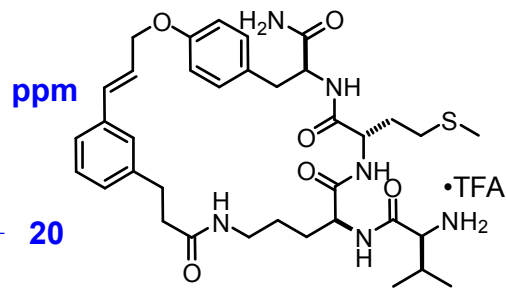
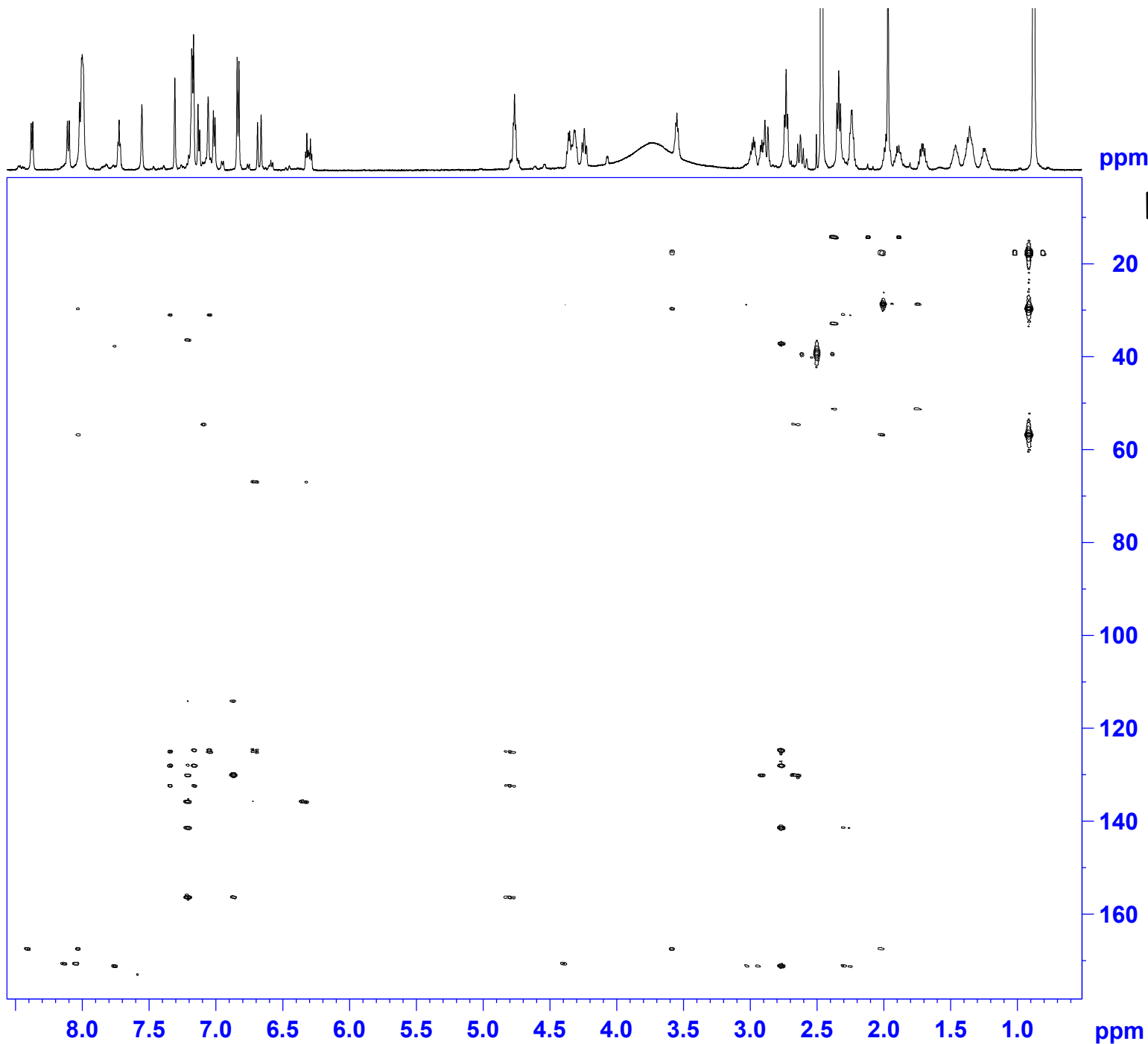


Current Data Parameters
 NAME KL-5-156C_AV600
 EXPNO 5
 PROCNO 1

F1 - Acquisition parameters
 TD 512
 SFO1 150.9134 MHz
 FIDRES 47.160427 Hz
 SW 160.000 ppm
 FnmODE Echo-Antiecho

F2 - Processing parameters
 SI 4096
 SF 600.130051 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 4096
 MC2 echo-antiecho
 SF 150.9029231 MHz
 WDW TRAP
 SSB 2
 LB 0 Hz
 GB 0



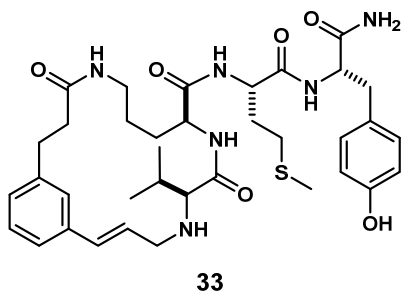
Current Data Parameters
 NAME KL-5-156C_AV600
 EXPNO 4
 PROCNO 1

F1 - Acquisition parameters
 TD 512
 SFO1 150.9156 MHz
 FIDRES 56.003849 Hz
 SW 190.000 ppm
 FnmODE QF

F2 - Processing parameters
 SI 4096
 SF 600.1300066 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 4096
 MC2 QF
 SF 150.9029181 MHz
 WDW USER
 SSB 3
 LB 0 Hz
 GB 0

Cyclic-Val-Orn-Met-Try (33):

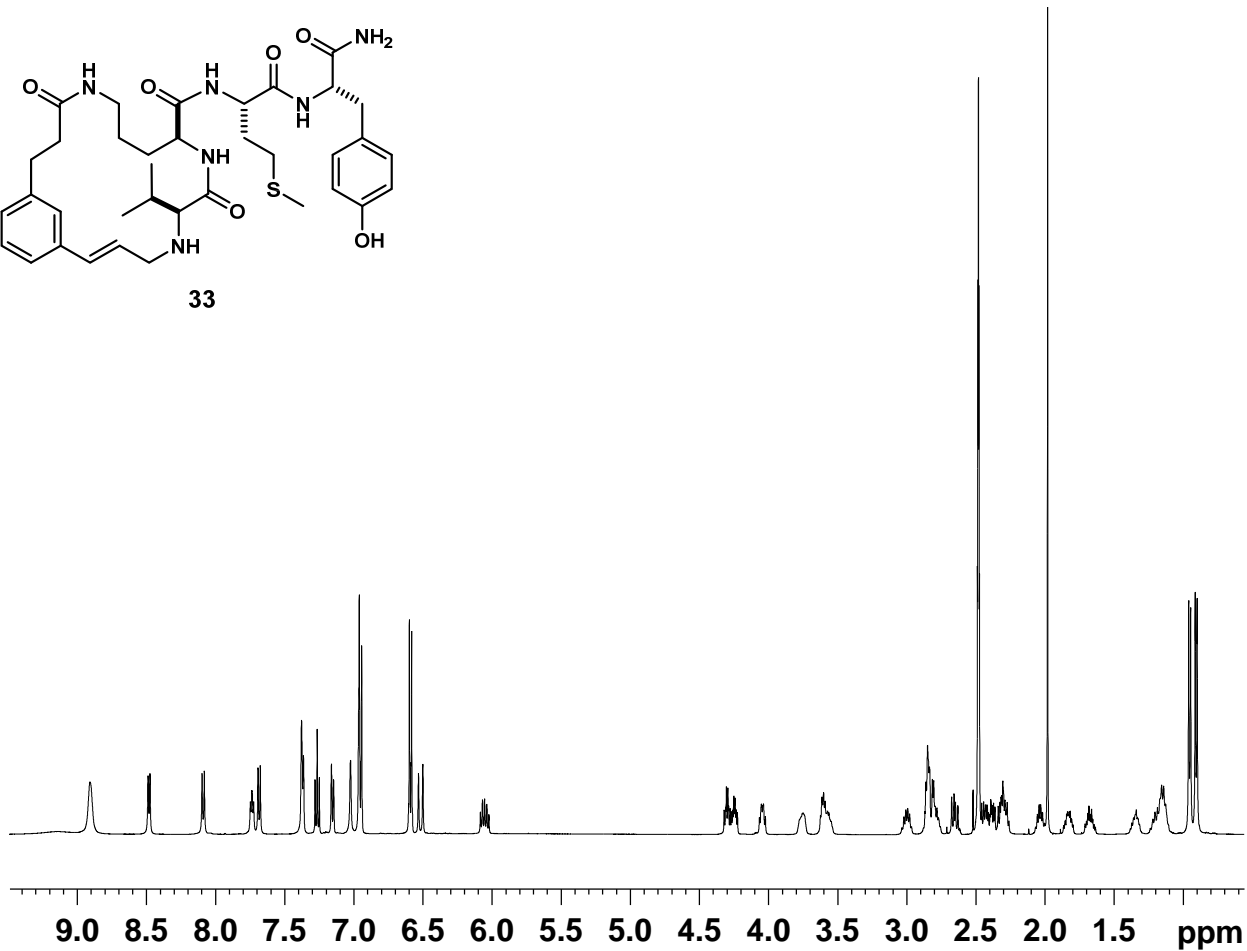


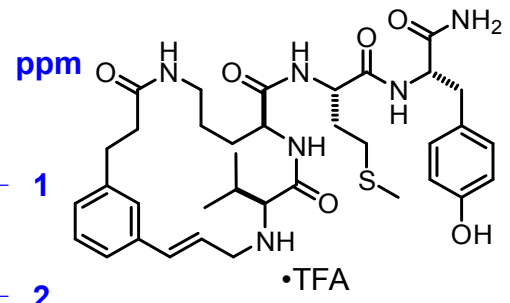
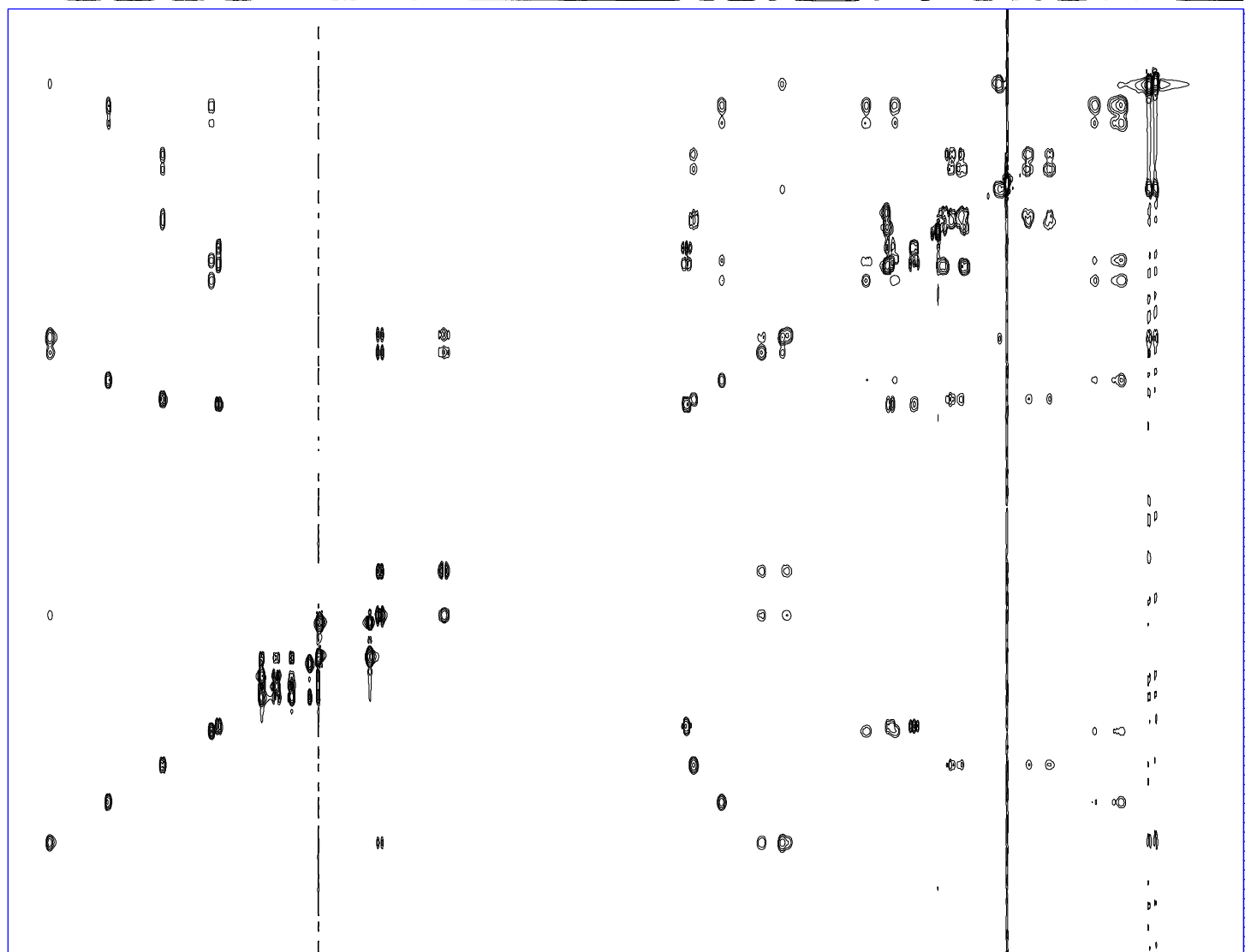
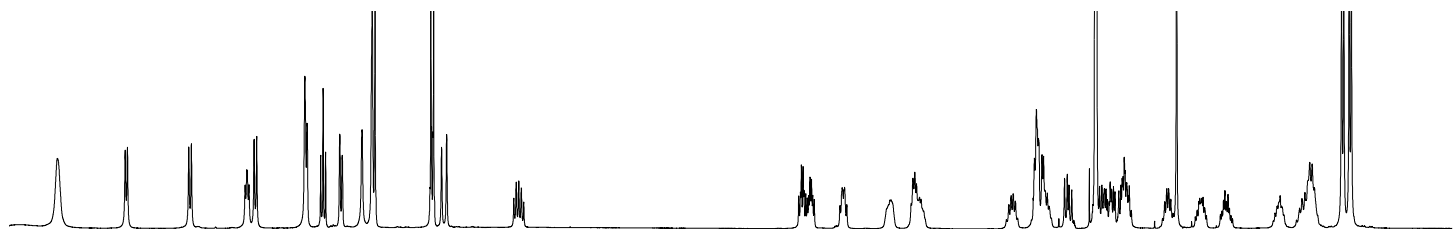
Current Data Parameters
NAME KL-5-156A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130410
Time 11.40
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 72.5
DW 50.000 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.1330008 MHz
NUC1 1H
P1 10.00 usec
PLW1 13.50000000 W

F2 - Processing parameters
SI 65536
SF 500.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





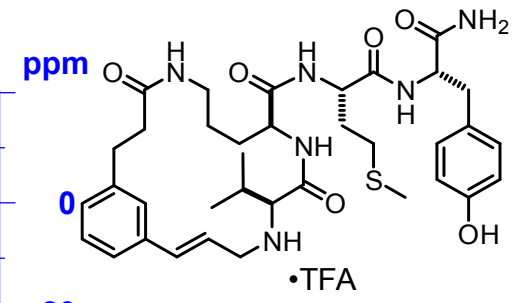
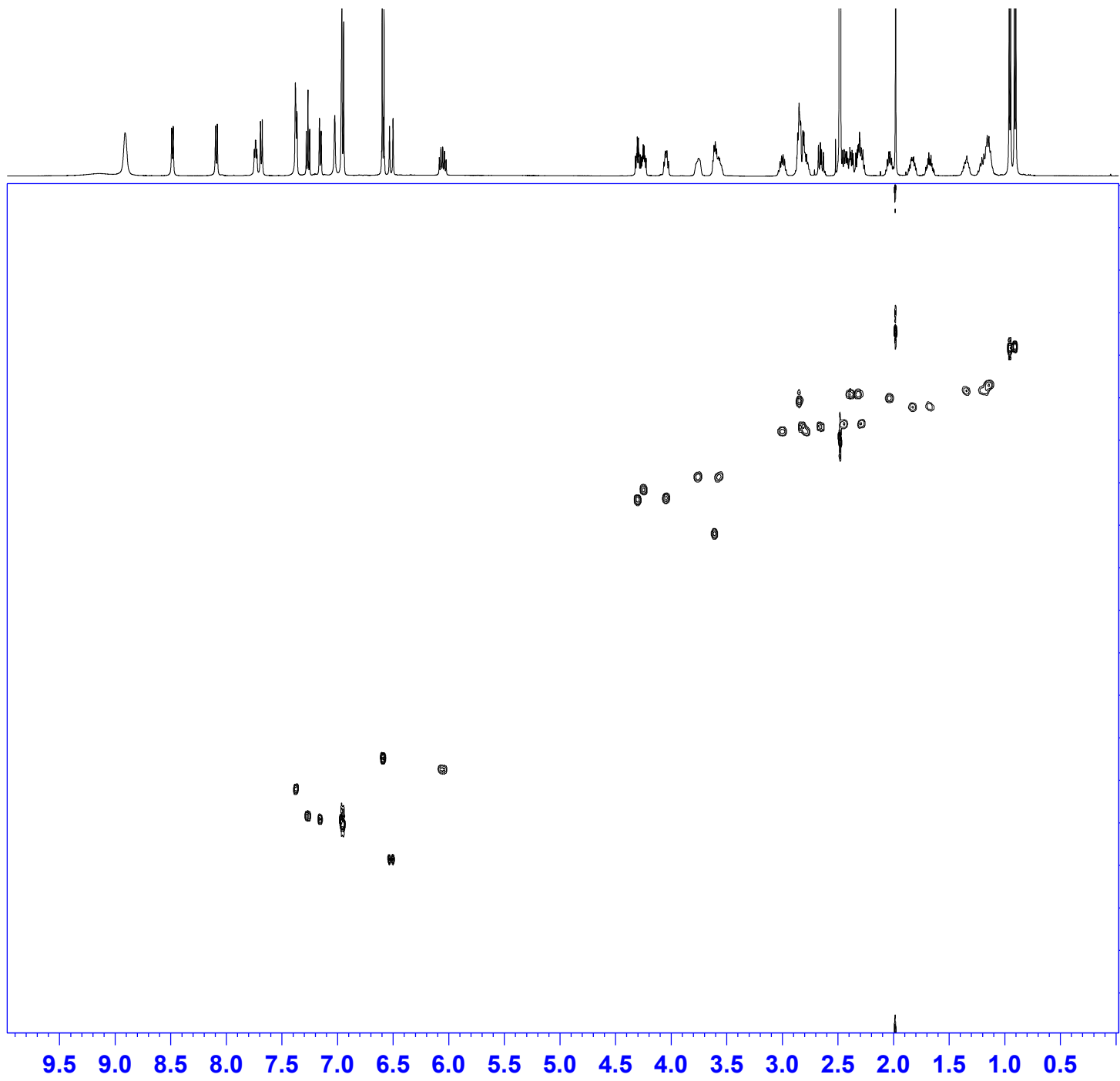
Current Data Parameters
NAME KL-5-156A
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130410
Time 12.16
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG mlevetgp.js
TD 2048
SOLVENT DMSO
NS 2
DS 8
SWH 6009.615 H:
FIDRES 2.934382 H:
AQ 0.1703936 s:
RG 37.94
DW 83.200 u:
DE 10.00 u:
TE 298.0 K
D0 0.00000300 s:
D1 2.00000000 s:
D9 0.06000000 s:
D11 0.03000000 s:
D12 0.00002000 s:
D16 0.00020000 s:
IN0 0.00016660 s:
L1 24

==== CHANNEL f1 =====
SFO1 500.1330008 MHz
NUC1 1H
P1 9.50 u:
P2 19.00 u:
P5 26.68 u:
P6 40.00 u:
P7 80.00 u:
P17 2500.00 u:
PLW1 13.5000000 W
PLW10 0.84375000 W

==== GRADIENT CHANNEL =====
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1 30.00 %

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

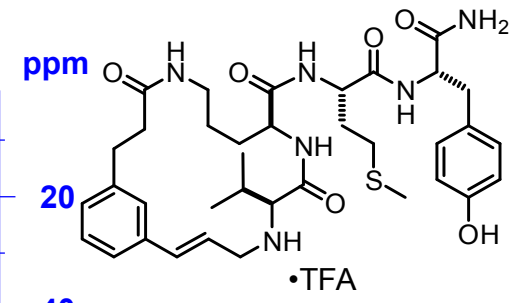
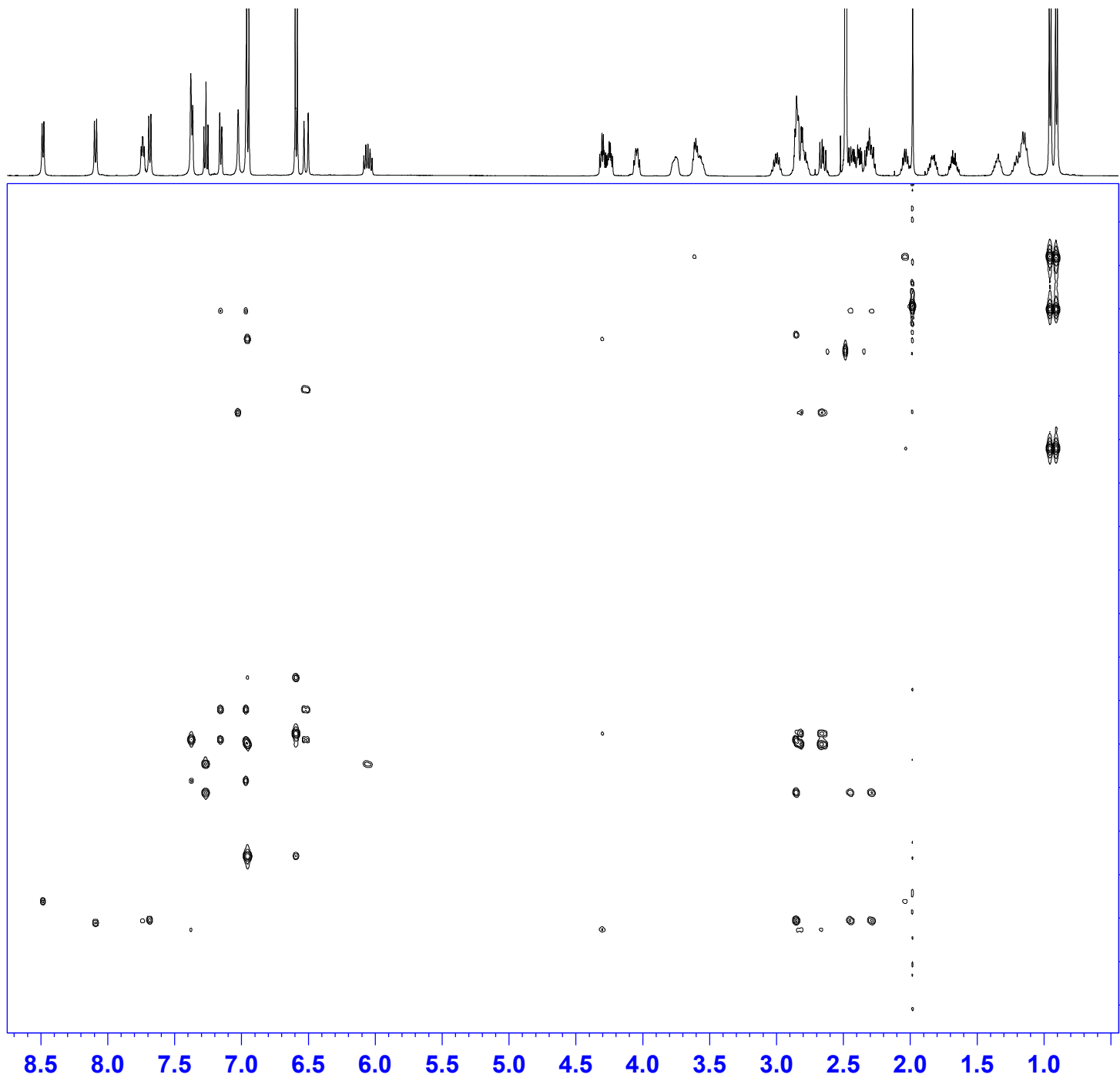


Current Data Parameters
 NAME KL-5-156A
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20130410
 Time 11.45
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hsqcedetgp
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 5000.000 H:
 FIDRES 2.441406 H:
 AQ 0.2048000 s:
 RG 202.91
 DW 100.000 u:
 DE 10.00 u:
 TE 298.0 K
 CNST2 145.0000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D4 0.00172414 s:
 D11 0.03000000 s:
 D13 0.00000400 s:
 D16 0.00020000 s:
 D21 0.00345000 s:
 IN0 0.00001990 s:
 ZGPTNS

==== CHANNEL f1 =====
 SFO1 500.1325007 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 P28 0 usec
 PLW1 13.50000000 W

==== CHANNEL f2 =====
 SFO2 125.7678496 MHz
 NUC2 13C
 CPDPRG[2] garp
 P3 9.63 u:
 P4 19.26 u:



Current Data Parameters
 NAME KL-5-156A
 EXPNO 5
 PROCNO 1

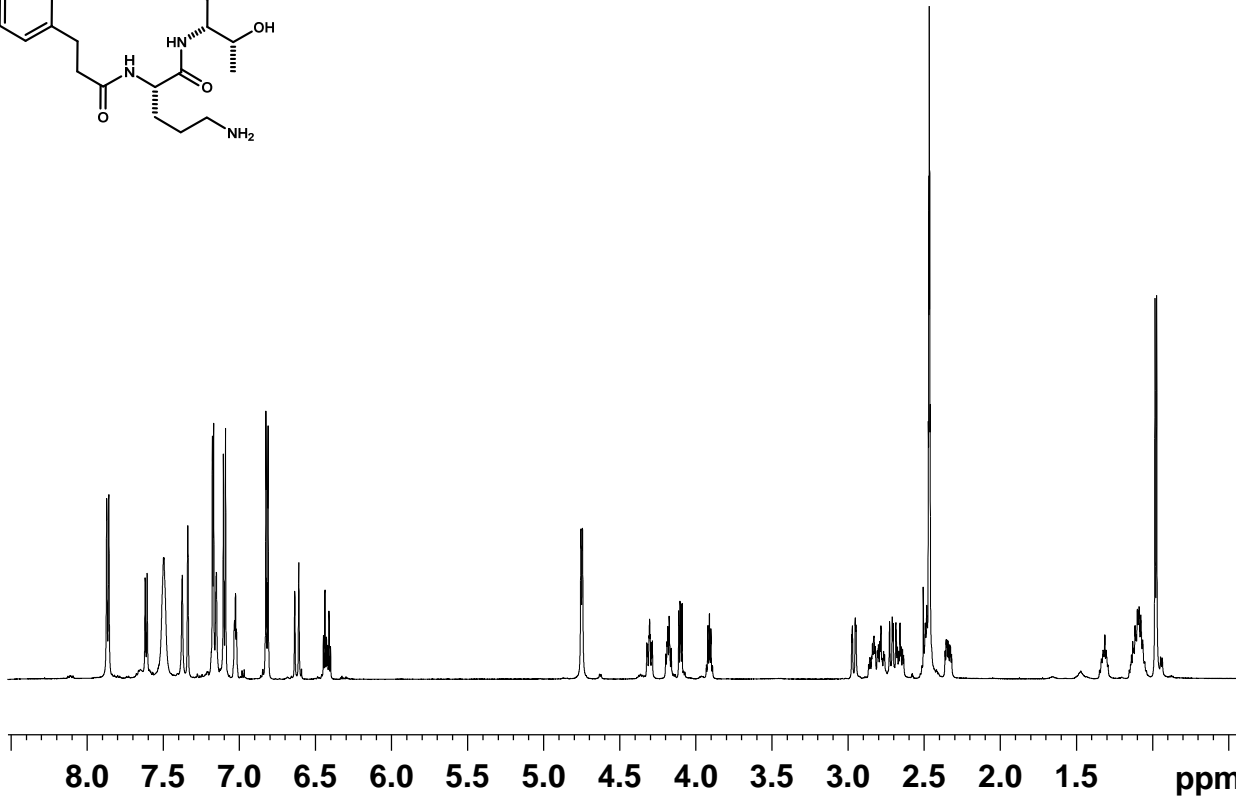
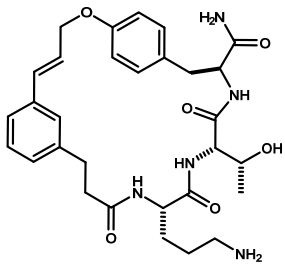
F2 - Acquisition Parameters
 Date_ 20130410
 Time 12.00
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 202.91
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 D0 0.00000300 s:
 D1 1.50000000 s:
 D6 0.07142857 s:
 D16 0.00020000 s:
 IN0 0.00001990 s:

===== CHANNEL f1 =====
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 PLW1 13.50000000 W

===== CHANNEL f2 =====
 SFO2 125.7703648 MHz
 NUC2 13C
 P3 9.63 u:
 PLW2 23.01399994 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100

Cyclic-Orn-Thr-Try (35):

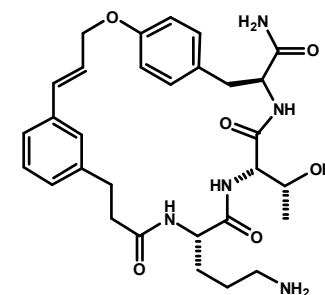
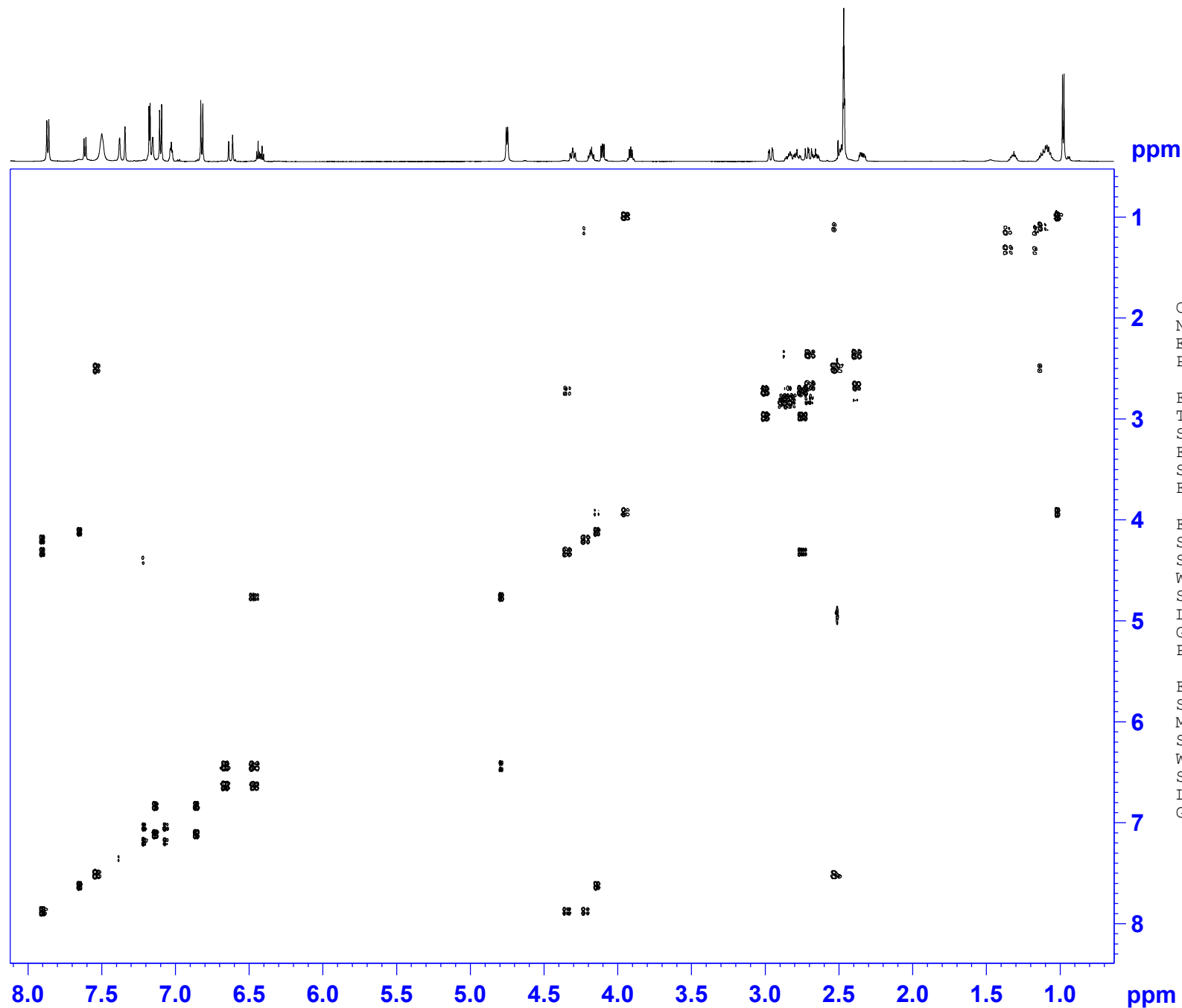


Current Data Parameters
NAME TR4-169A_2
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130428
Time 18.14
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG zgpr
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 64
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D12 0.00002000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.70 usec
PL1 -2.00 dB
PL9 52.24 dB
PL1W 39.81071854 W
PL9W 0.00014997 W
SFO1 600.1321531 MHz

F2 - Processing parameters
SI 65536
SF 600.1300273 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ppm

1

2

3

4

5

6

7

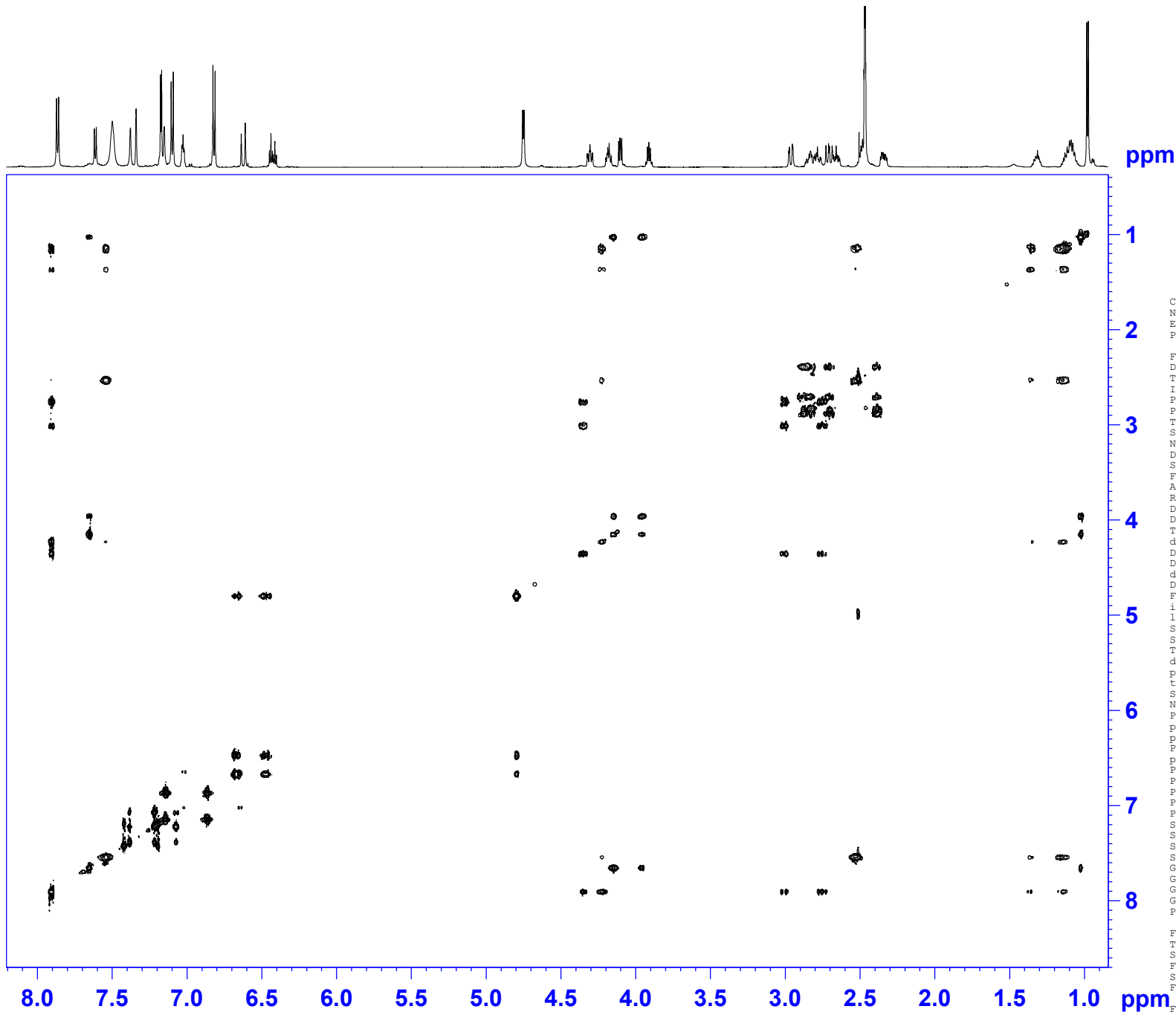
8

Current Data Parameters
 NAME TR4-169A_2
 EXPNO 5
 PROCNO 1

F1 - Acquisition parameters
 TD 512
 SFO1 600.133 MHz
 FIDRES 11.737530 Hz
 SW 10.014 ppm
 FnMODE States-TPPI

F2 - Processing parameters
 SI 4096
 SF 600.130014 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 4096
 MC2 States-TPPI
 SF 600.1300177 MHz
 WDW TRAP
 SSB 2
 LB 0 Hz
 GB 0



ppm

1

2

3

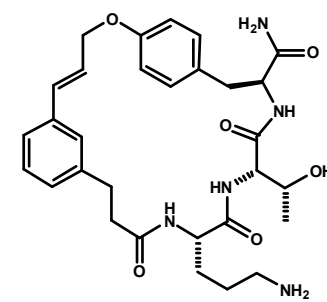
4

5

6

7

8



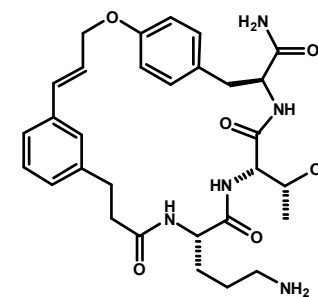
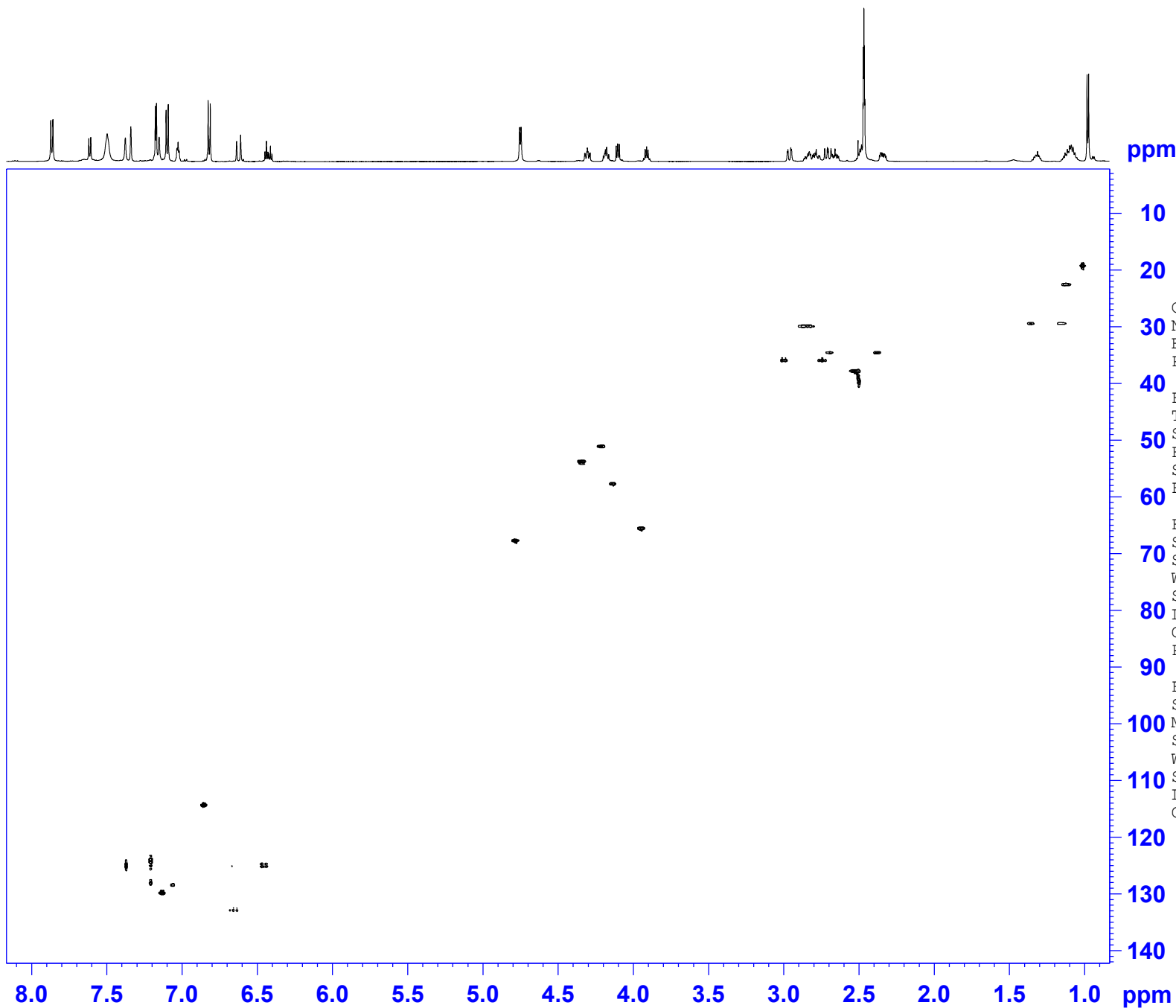
```

Current Data Parameters
NAME      TR4-169A_2
EXPNO    6
PROCNO   1

F2 - Acquisition Parameters
Date_    20130428
Time     18.35
INSTRUM  av600
PROBHD   5 mm TBI5
PULPROG  mlevsgpph
TD       2048
SOLVENT  DMSO
NS       2
DS       16
SWH      6009.615 Hz
FIDRES   2.934382 Hz
AQ       0.1703936 sec
RG       812.7
DW       83.200 usec
DE       6.50 usec
TE       298.0 K
d0       -0.00002618 sec
D1       1.00000000 sec
D9       0.06000000 sec
d12      0.00002000 sec
D16      0.00020000 sec
FACTOR1  4
in0      0 sec
l1       24
SCALEF   6
ST1CNT   128
TAU      0.00006668 sec
d0orig   -0.00002618 sec
phloop   0
tiloop   0
SFO1     600.1330006 MHz
NUC1     1H
P1       9.70 usec
p2       19.40 usec
p5       26.68 usec
P6       40.00 usec
p7       80.00 usec
P12      3000.00 usec
P17      2500.00 usec
PLW0     -1.00000000 W
PLW1     -1.00000000 W
PLW10    -1.00000000 W
SPNAM[1] Squa100.1000
SPOAL1   1.000
SPOFFS1  -1175.04 Hz
SPW1     0 W
GPNAM[1] SINE.100
GPNAM[2] SINE.100
GPZ1     31.00 %
GPZ2     11.00 %
P16      1000.00 usec

F1 - Acquisition parameters
TD       256
SFO1     600.133 MHz
FIDRES   23.475060 Hz
SW       10.014 ppm
FnMODE   States-TPPI

F2 - Processing parameters
SI       4096
SF       600.1300000 MHz
WDW      QSINE
SSB      2.5
LB       0 Hz
GB       0
  
```



ppm

10

20

Current Data Parameters

30 NAME TR4-169A_2

EXPNO 7

PROCNO 1

40 F1 - Acquisition parameters

TD 512

50 SFO1 150.9134 MHz

FIDRES 47.160427 Hz

SW 160.000 ppm

60 FnmODE Echo-Antiecho

F2 - Processing parameters

SI 4096

70 SF 600.1300051 MHz

WDW EM

SSB 0

80 LB 1.00 Hz

GB 0

PC 1.40

90 F1 - Processing parameters

SI 4096

100 MC2 echo-antiecho

SF 150.9029231 MHz

WDW SINE

110 SSB 2

LB 0 Hz

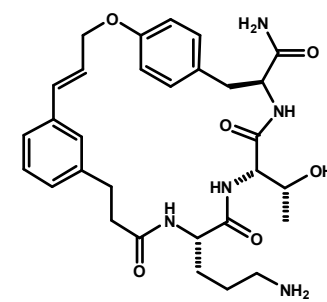
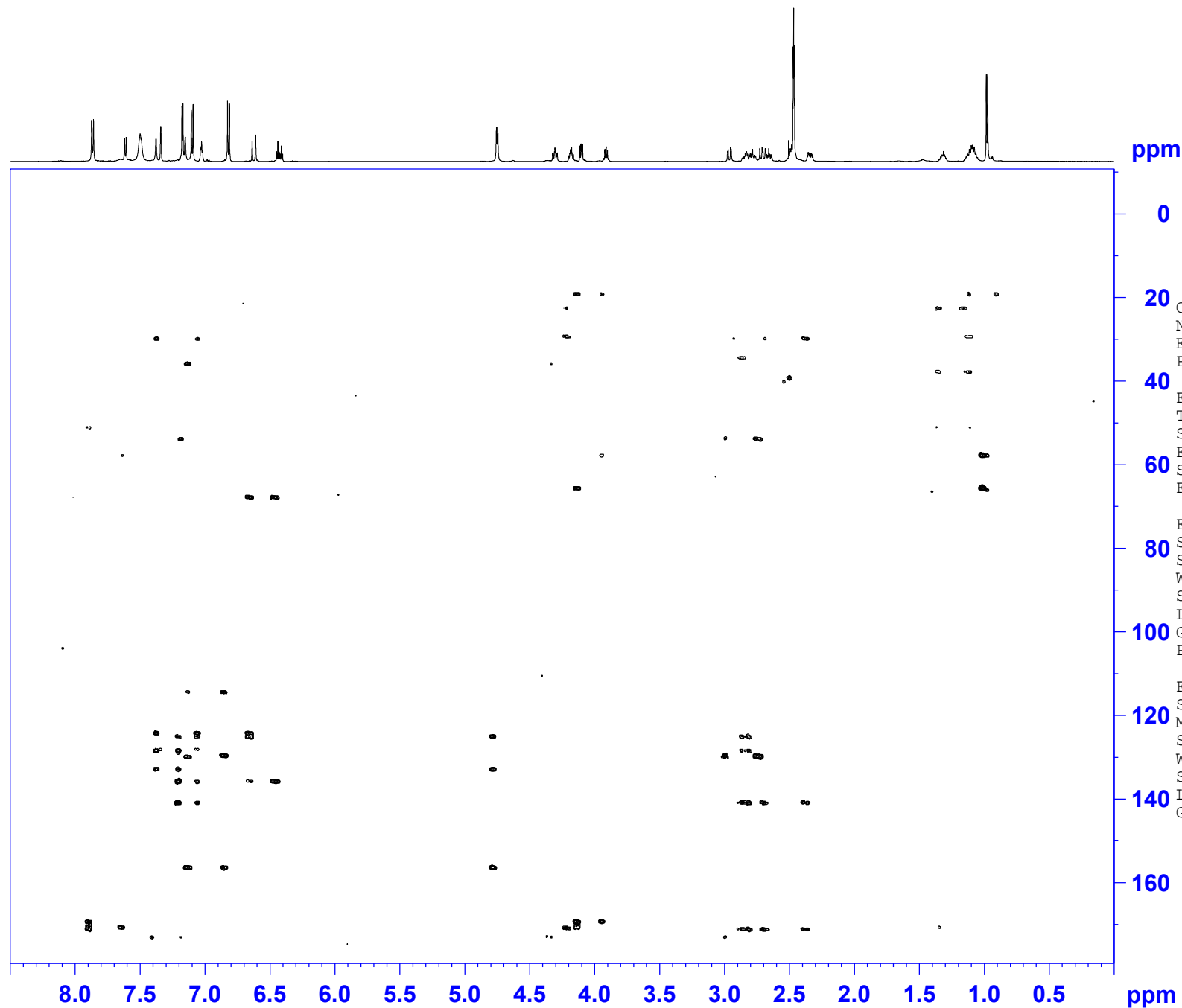
GB 0

120

130

140

ppm



ppm

0

20

40

60

80

100

120

140

160

ppm

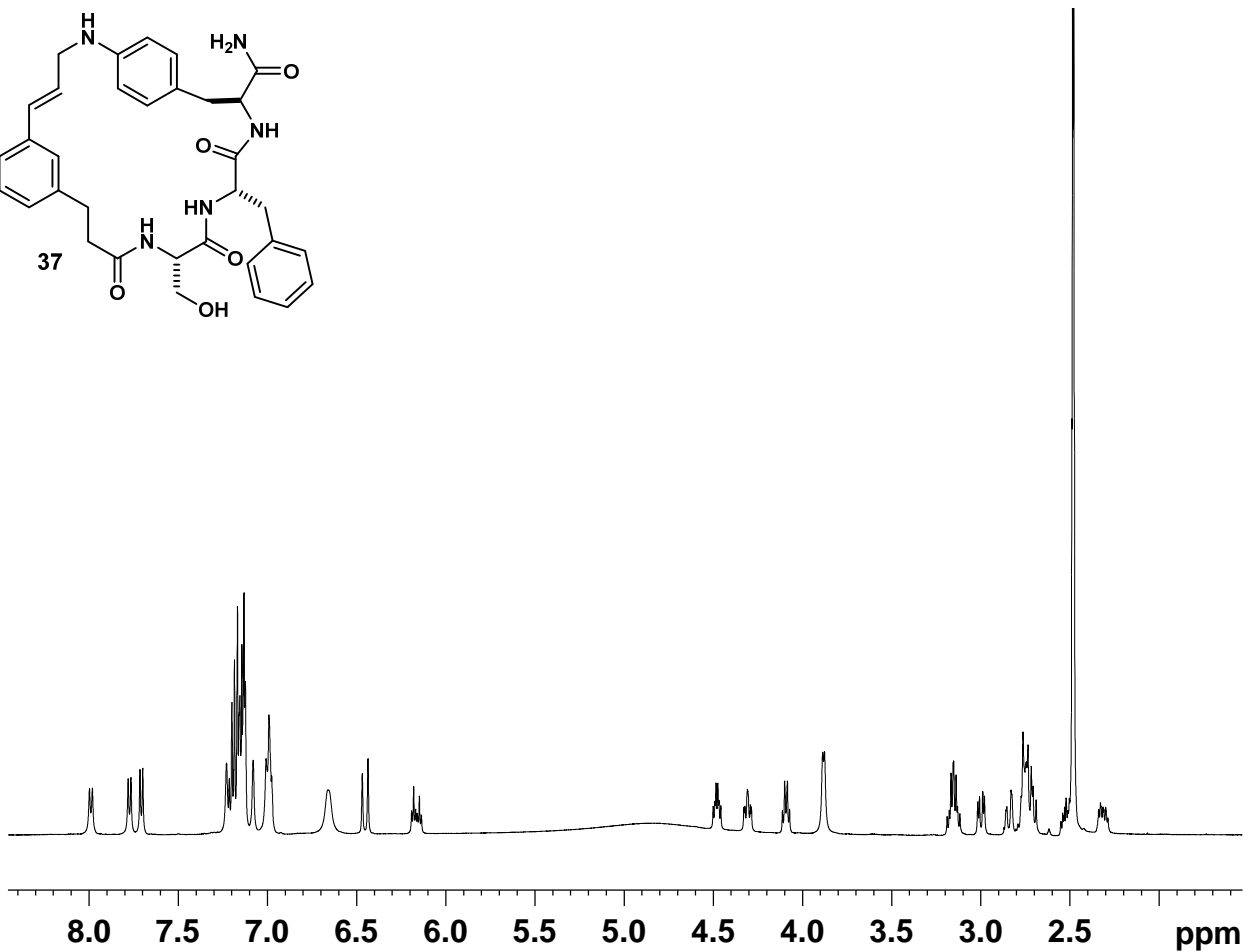
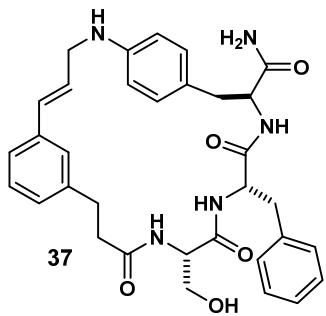
Current Data Parameters
 NAME TR4-169A_2
 EXPNO 8
 PROCNO 1

F1 - Acquisition parameters
 TD 512
 SFO1 150.9156 MHz
 FIDRES 56.003849 Hz
 SW 190.000 ppm
 FnMODE QF

F2 - Processing parameters
 SI 4096
 SF 600.130066 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 4096
 MC2 QF
 SF 150.9029181 MHz
 WDW QSINE
 SSB 1
 LB 0 Hz
 GB 0

Cyclic-Ser-Phe-Phe(4-NH₂) (37):

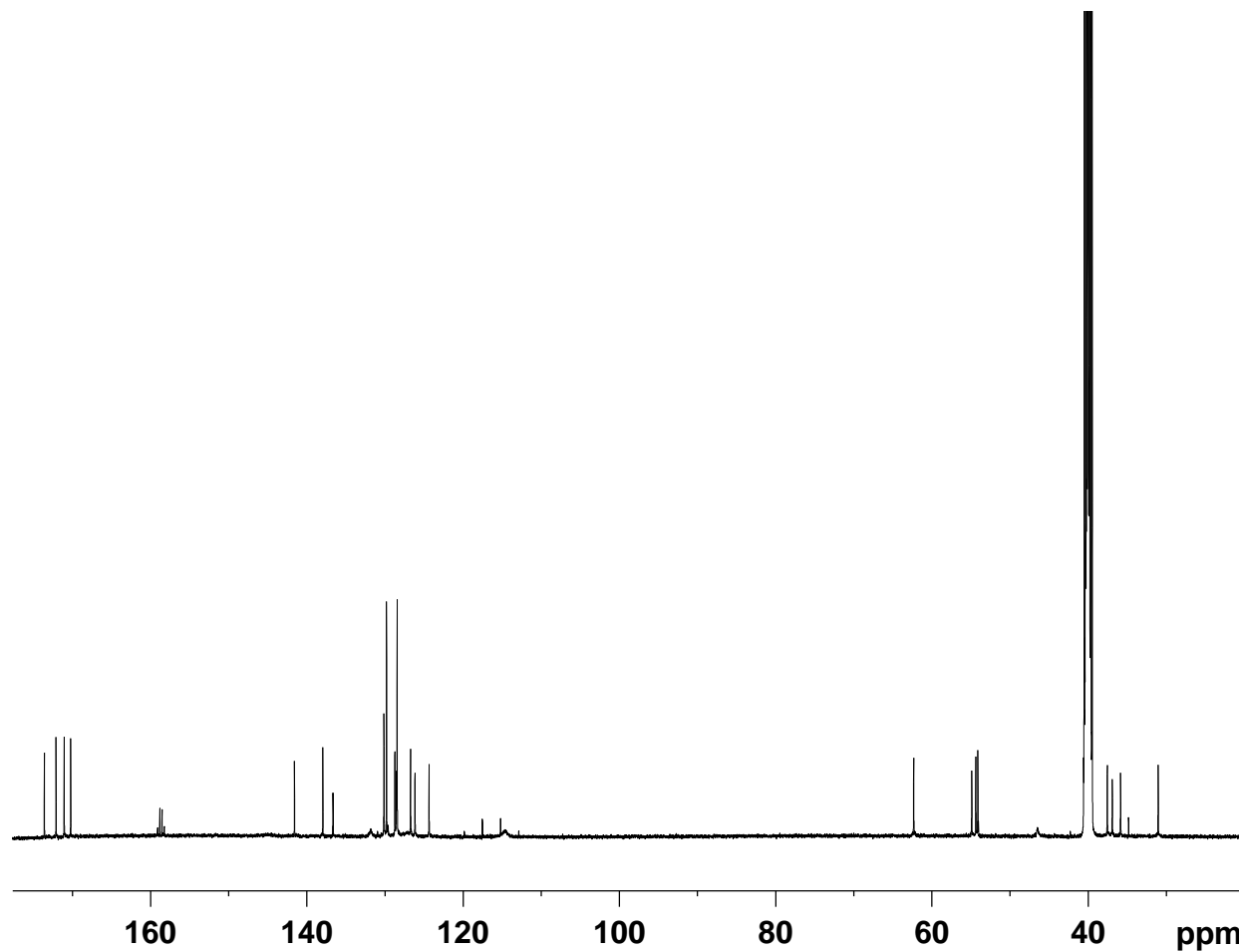


```
Current Data Parameters
NAME          KL-5-10
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20120815
Time          12.06
INSTRUM       av500
PROBHD        5 mm DCH 13C-1
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG            202.91
DW            50.000 usec
DE            10.00 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1
```

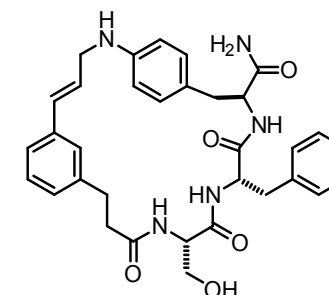
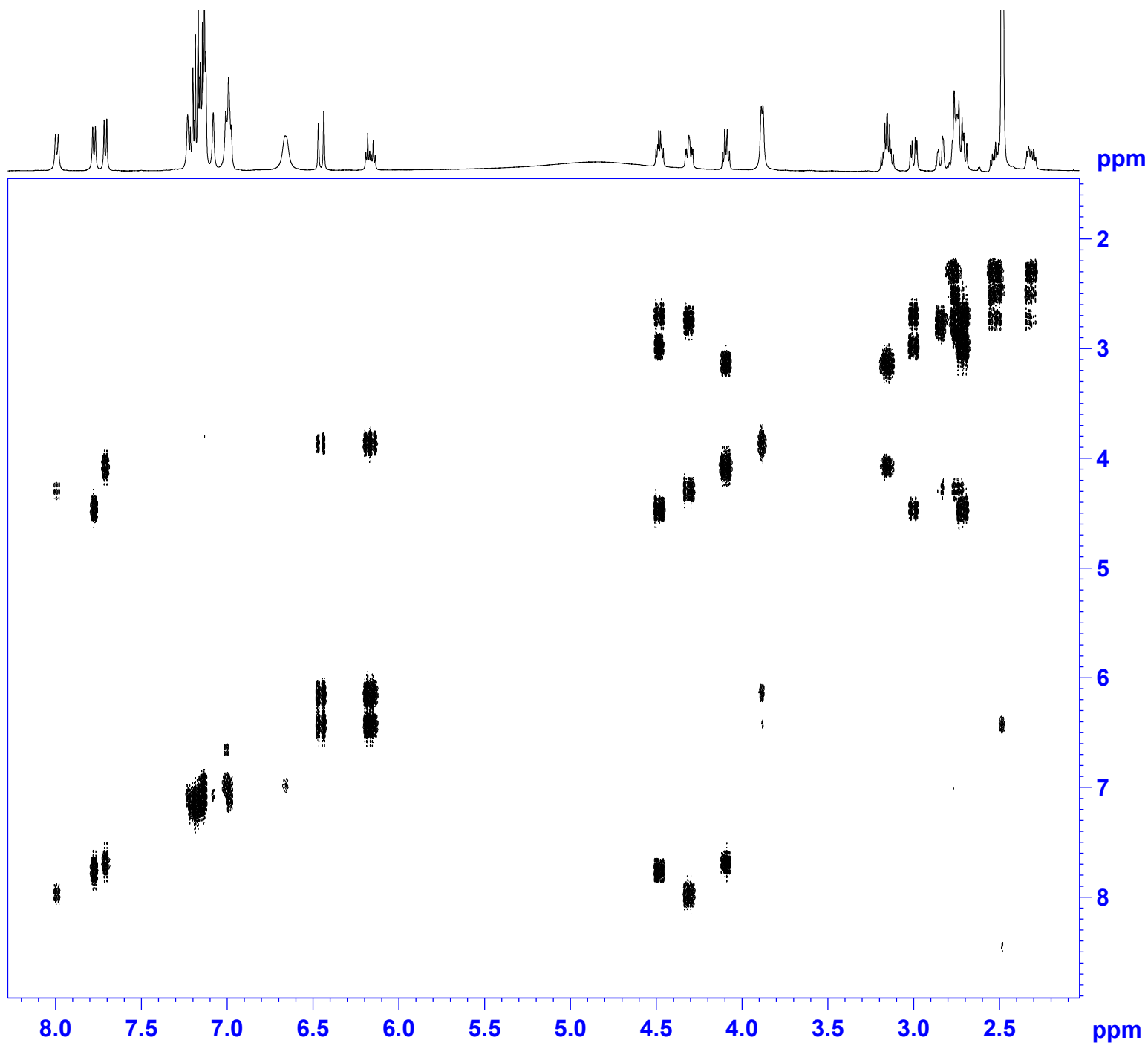
```
===== CHANNEL f1 =====
NUC1          1H
P1            10.00 usec
PLW1          13.5000000 W
SFO1          500.1330008 MHz
```

```
F2 - Processing parameters
SI            65536
SF            500.1300146 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



```
Current Data Parameters
NAME          KL-5-10
EXPNO         12
PROCNO        1

F2 - Processing parameters
SI            131072
SF            125.7577892 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

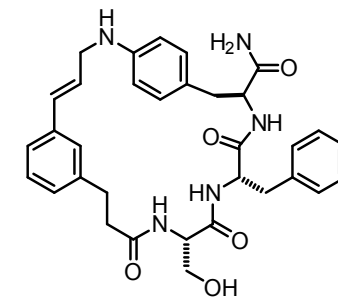
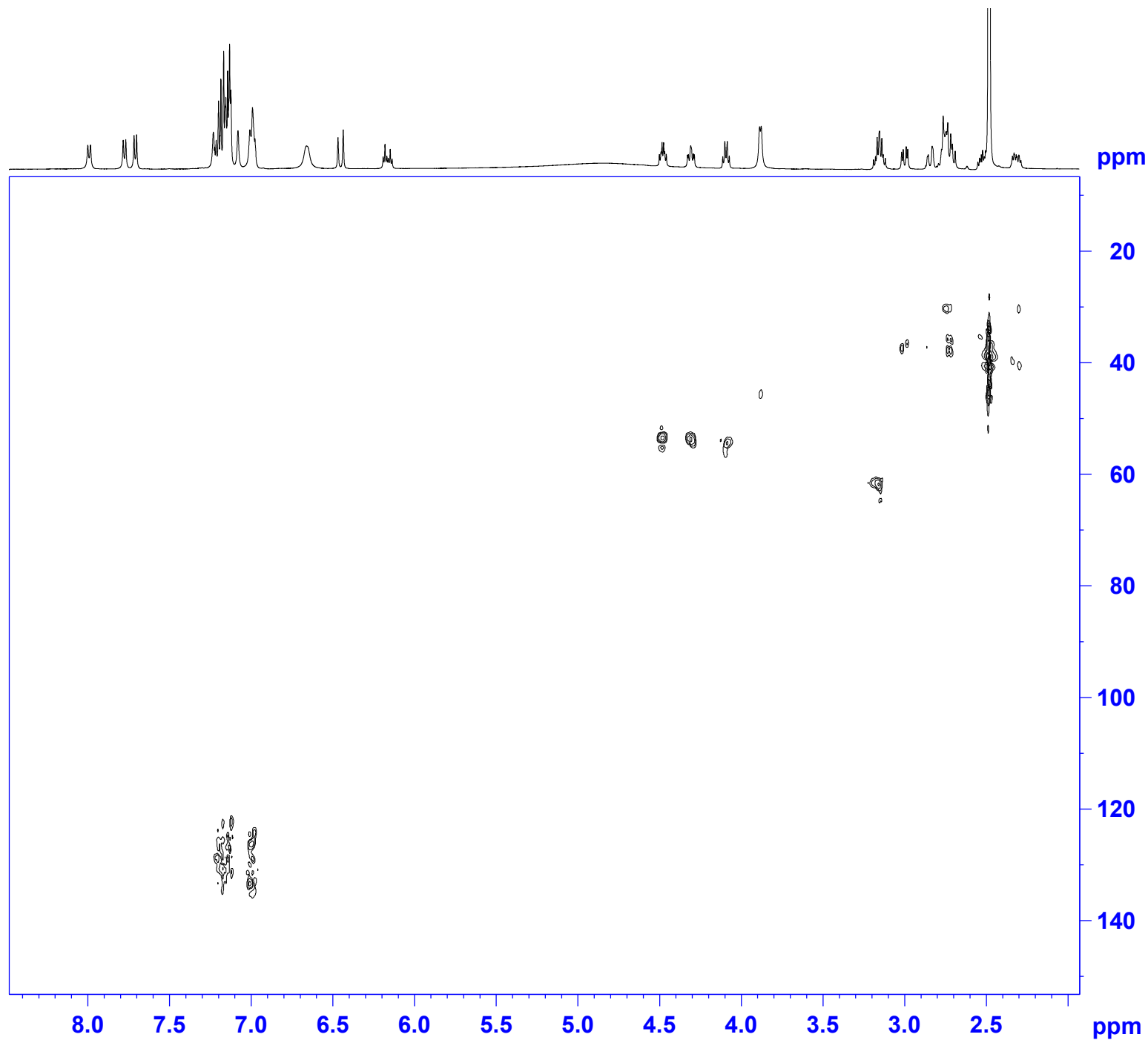


Current Data Parameters
 NAME KL-5-10
 EXPNO 3
 PROCNO 1

F1 - Acquisition parameters
 TD 256
 SFO1 500.1328 MHz
 FIDRES 19.536423 Hz
 SW 10.000 ppm
 FnMODE States-TPPI

F2 - Processing parameters
 SI 2048
 SF 500.1300135 MHz
 WDW SINE
 SSB 1
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 States-TPPI
 SF 500.1300216 MHz
 WDW SINE
 SSB 1
 LB 0 Hz
 GB 0



Current Data Parameters

NAME KL-5-10
EXPNO 4
PROCNO 1

F1 - Acquisition parameters

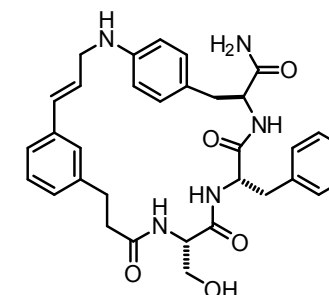
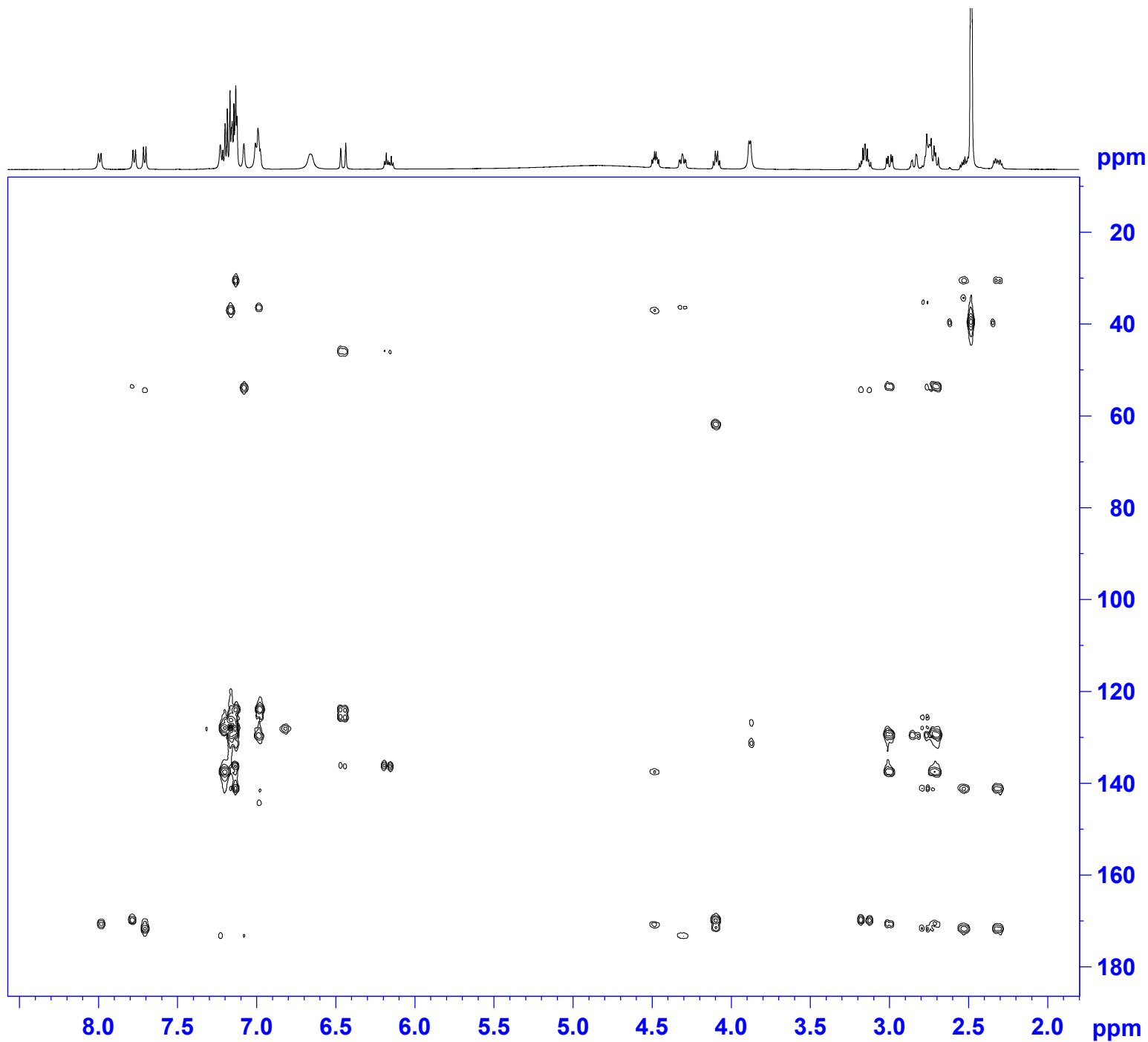
TD 256
SFO1 125.7678 MHz
FIDRES 98.255890 Hz
SW 200.000 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters

SI 2048
SF 500.1300135 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters

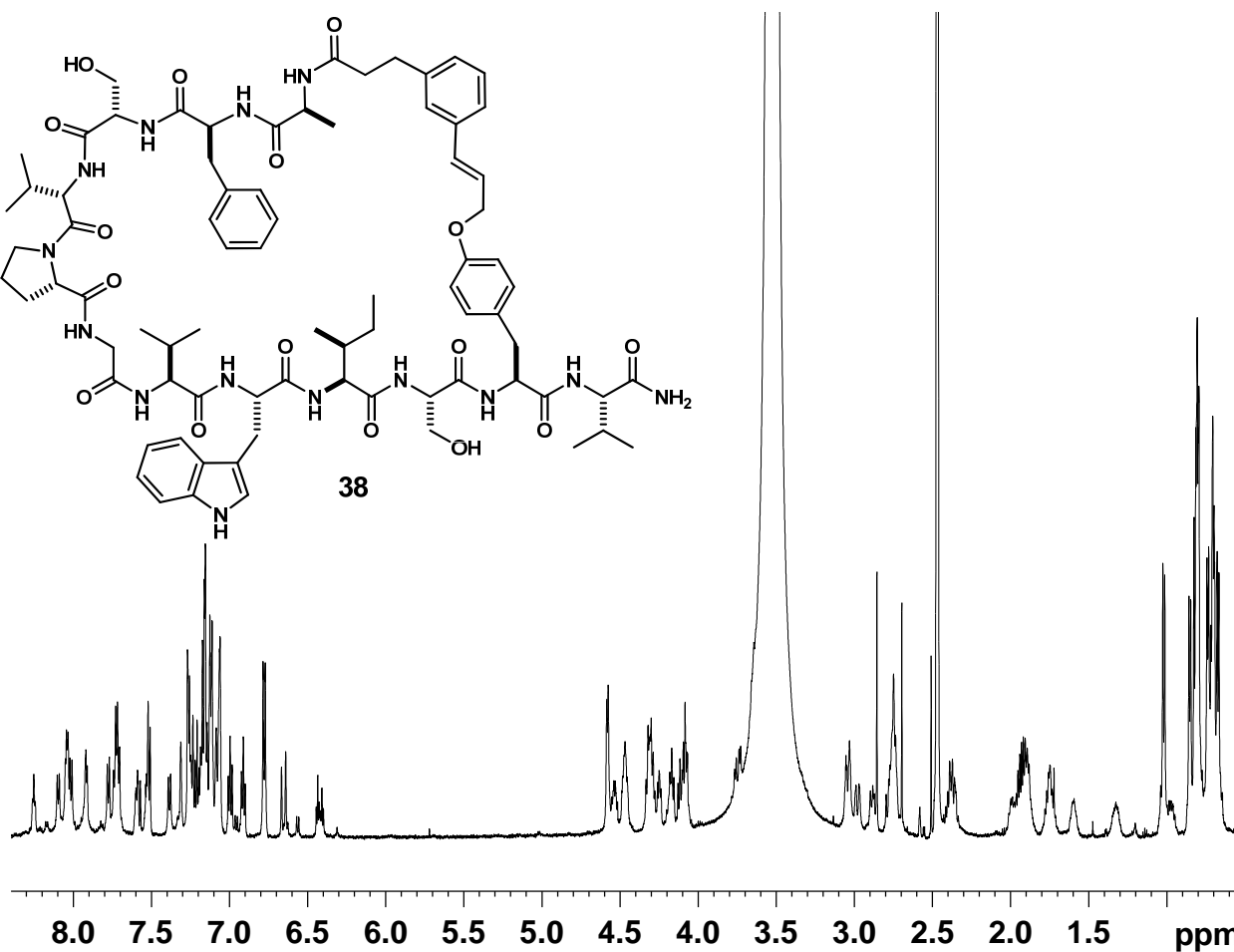
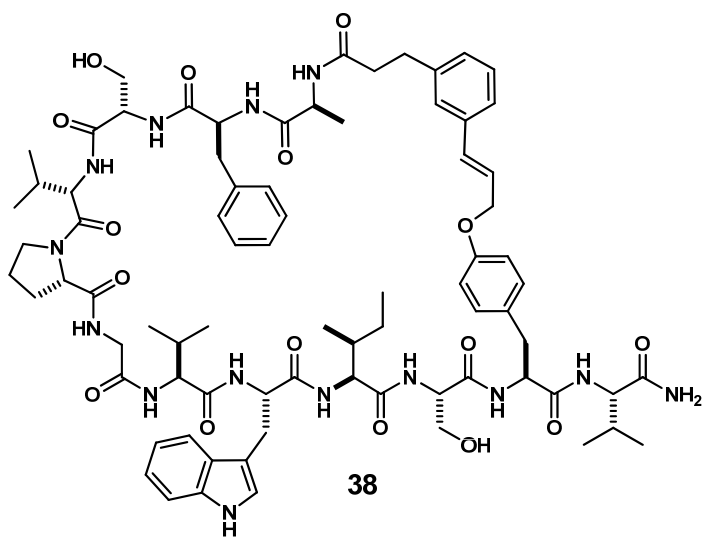
SI 2048
MC2 echo-antiecho
SF 125.7578472 MHz
WDW TRAP
SSB 2
LB 0 Hz
GB 0



Current Data Parameters
 NAME KL-5-10
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120816
 Time 19.26
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG hmbcgp12ndqf
 TD 2048
 SOLVENT DMSO
 NS 4
 DS 16
 SWH 6009.615 H:
 FIDRES 2.934382 H:
 AQ 0.1703936 s:
 RG 202.91
 DW 83.200 u:
 DE 10.00 u:
 TE 298.0 K
 CNST6 120.000000
 CNST7 160.000000
 CNST13 7.000000
 d0 0.00000300 s:
 D1 1.50000000 s:
 d6 0.07142857 s:
 D16 0.00020000 s:
 DELTA1 0.00296667 s:
 DELTA2 0.00192500 s:
 DELTA3 0.07022458 s:
 in0 0 sec
 ST1CNT 256
 d0orig 0.00000300 s:
 phloop 0
 t1loop 0
 SFO1 500.1330008 MHz
 NUC1 1H
 P1 10.00 u:
 p2 20.00 u:
 PLW1 13.50000000 W
 SFO2 125.7703648 MHz
 NUC2 13C
 P3 9.63 u:
 PLW2 23.01399994 W
 GPNAM[1] SMSQ10.100

Cyclic-Ala-Phe-Ser-Val-Pro-Gly-Val-Trp-Ile-Ser-Tyr-Val (38):

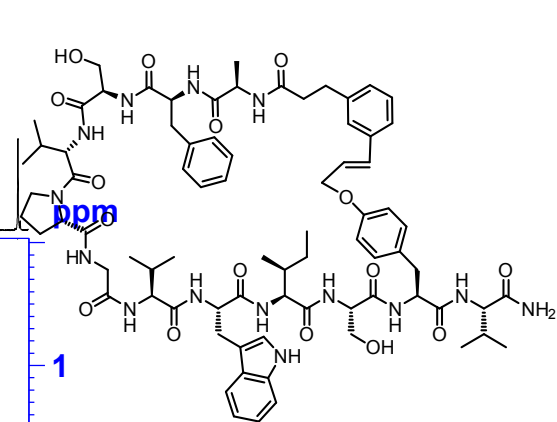
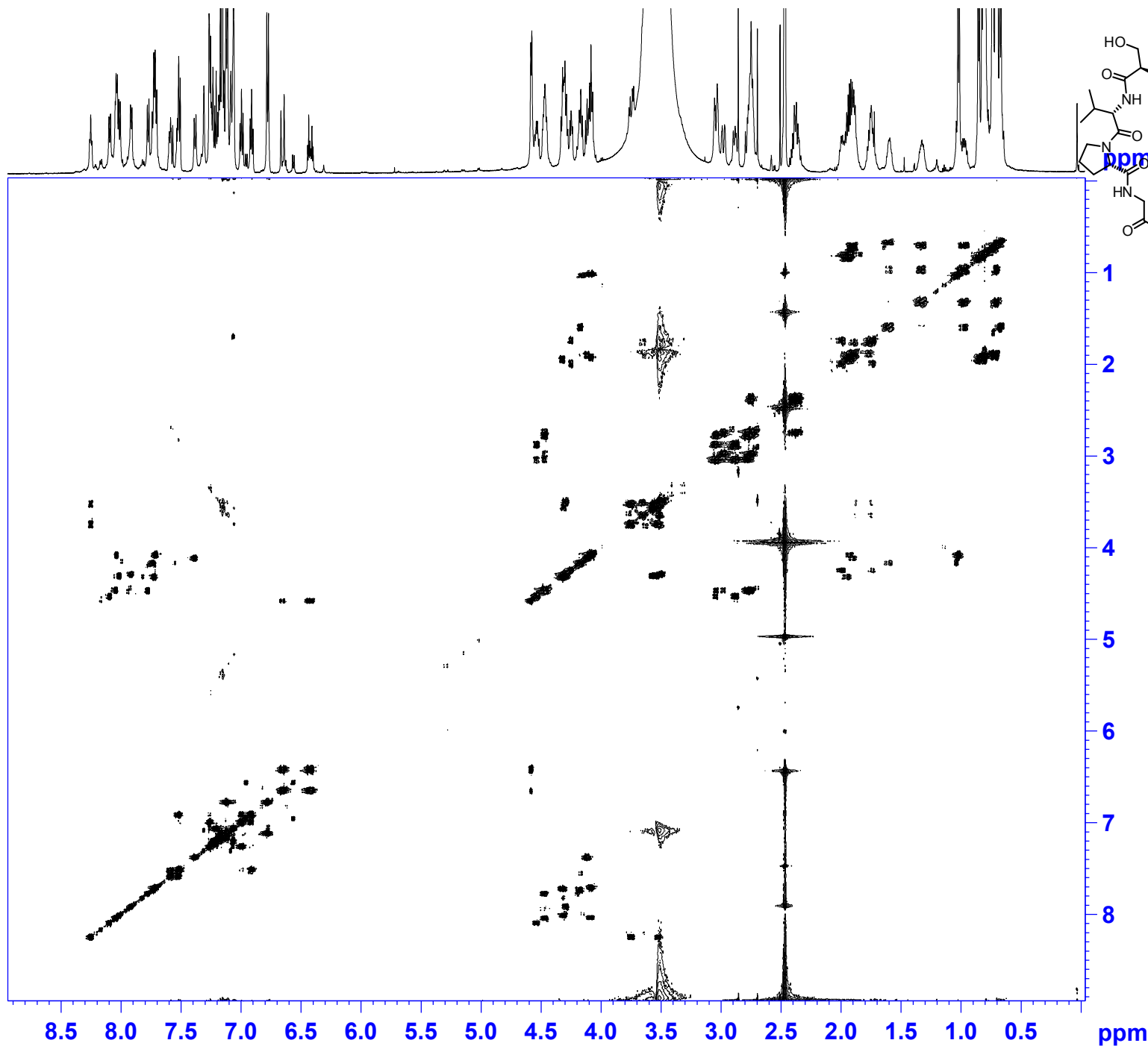


Current Data Parameters
NAME KL-4-44
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111006
Time 18.36
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 12376.237 Hz
FIDRES 0.188846 Hz
AQ 2.6476543 sec
RG 181
DW 40.400 usec
DE 6.50 usec
TE 295.8 K
DL 2.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.10 usec
PL1 -2.00 dB
PL1W 39.81071854 W
SFO1 600.1336008 MHz

F2 - Processing parameters
SI 65536
SF 600.1300273 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

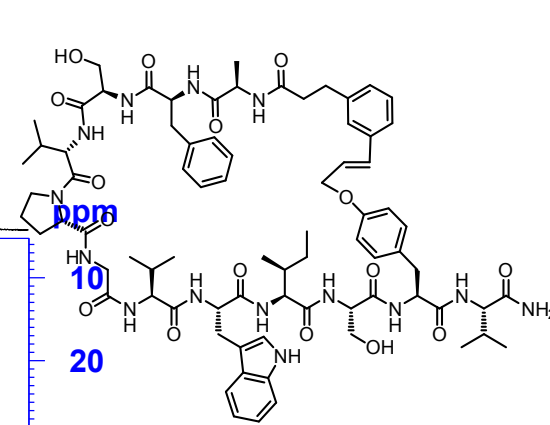
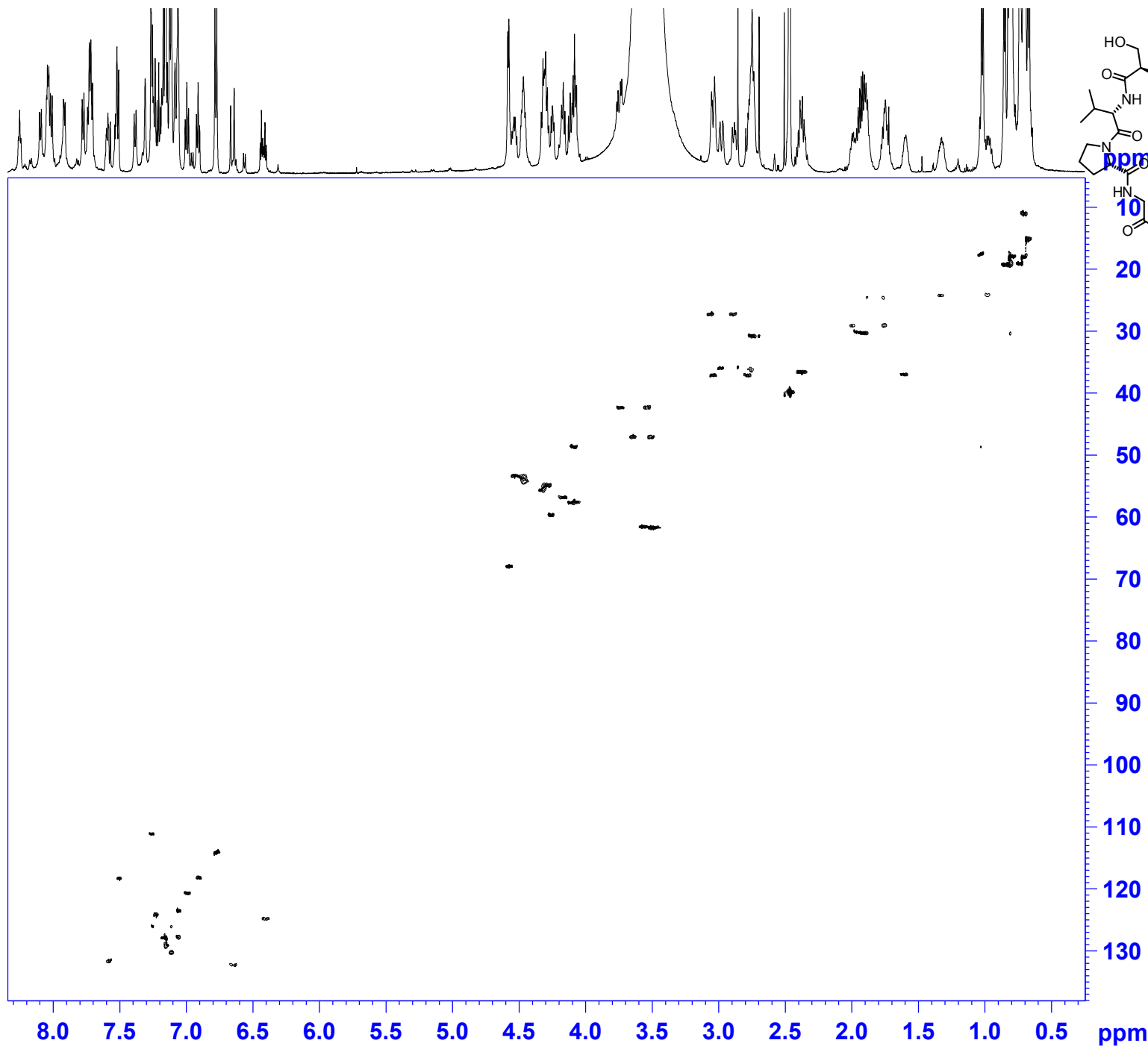


Current Data Parameters
 NAME KL-4-44
 EXPNO 2
 PROCNO 1

F1 - Acquisition parameters
 TD 512
 SFO1 600.1327 MHz
 FIDRES 10.523297 Hz
 SW 8.978 ppm
 FnmODE States-TPPI

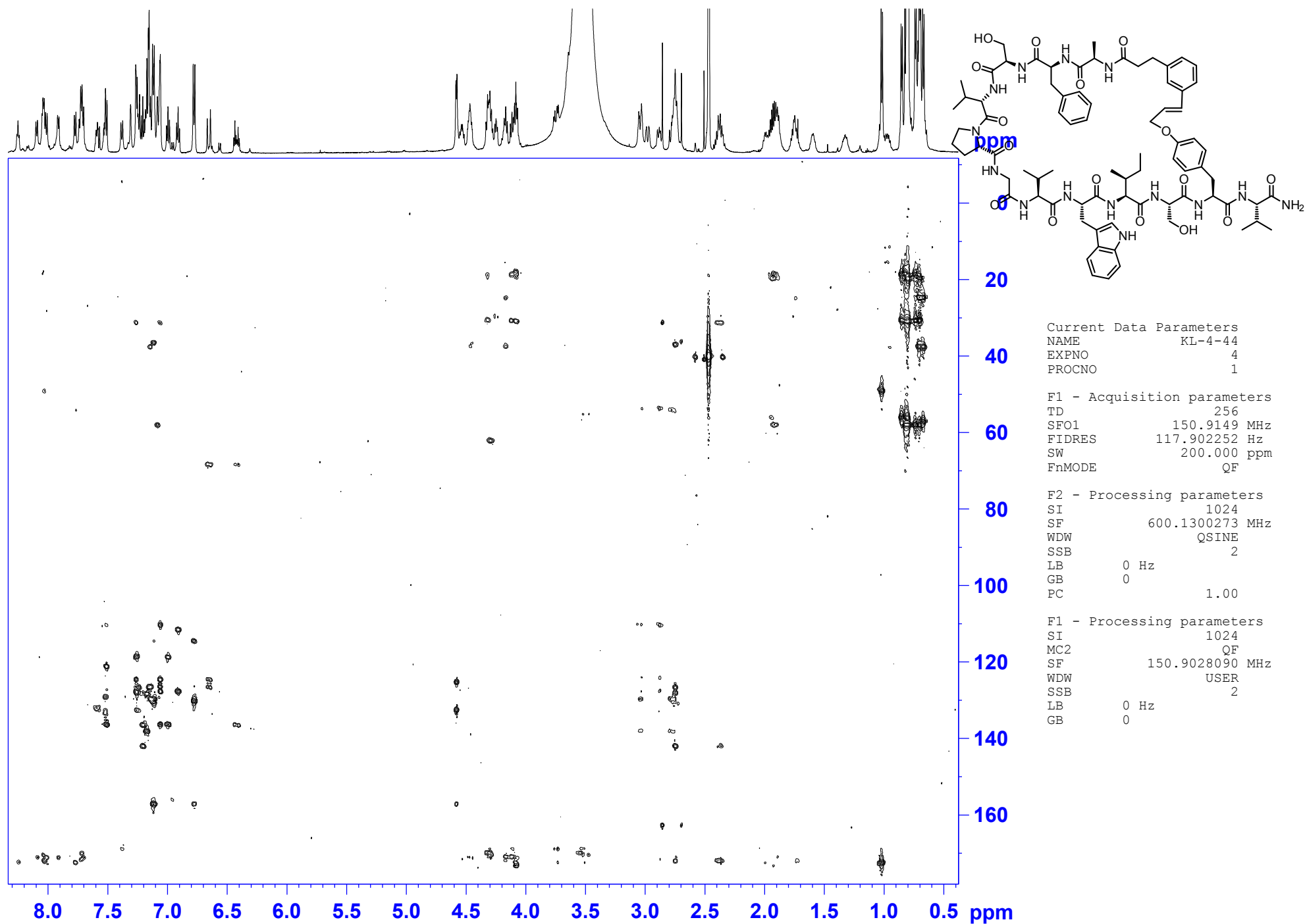
F2 - Processing parameters
 SI 2048
 SF 600.1300273 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 2048
 MC2 States-TPPI
 SF 600.1300273 MHz
 WDW TRAP
 SSB 2
 LB 0 Hz
 GB 0

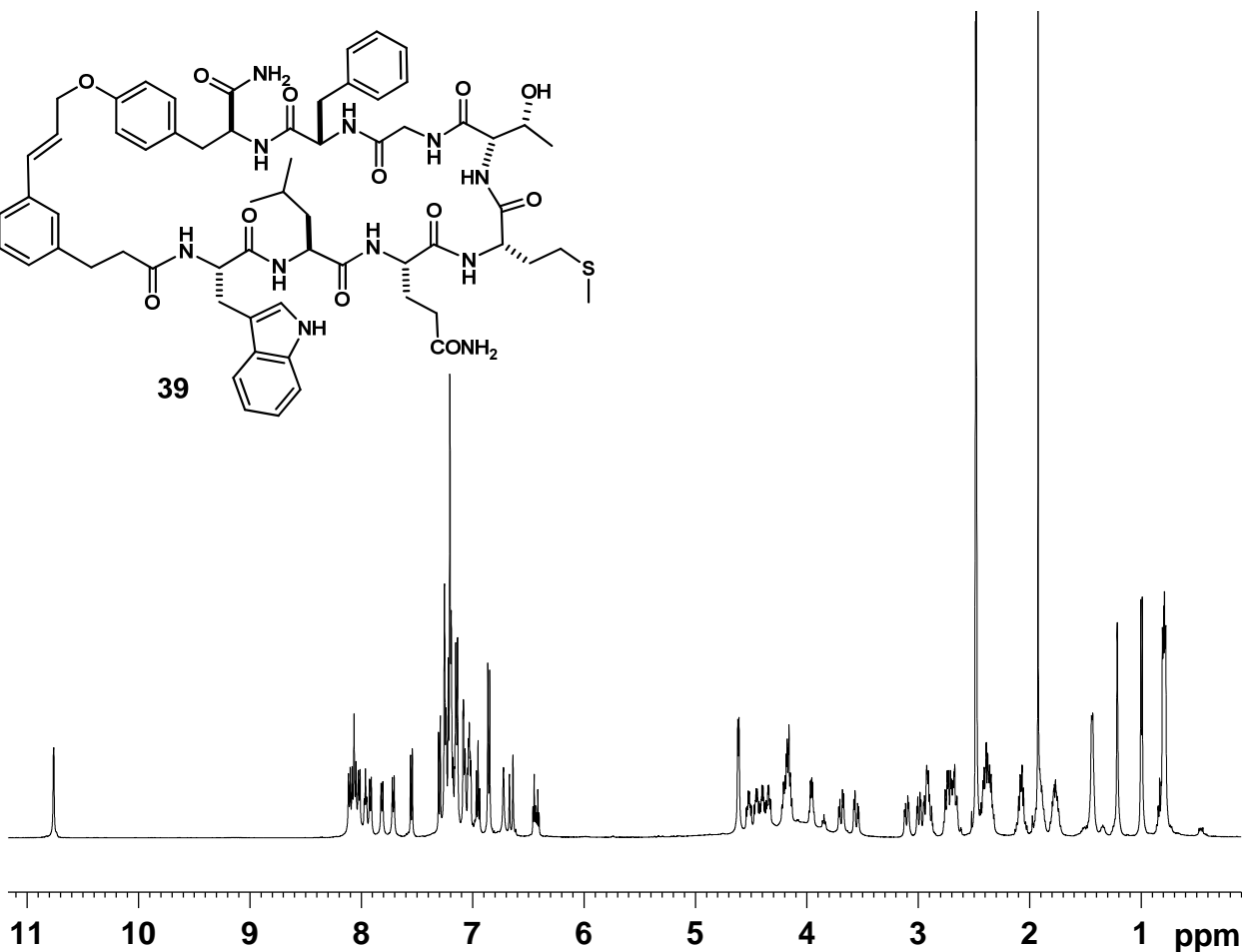
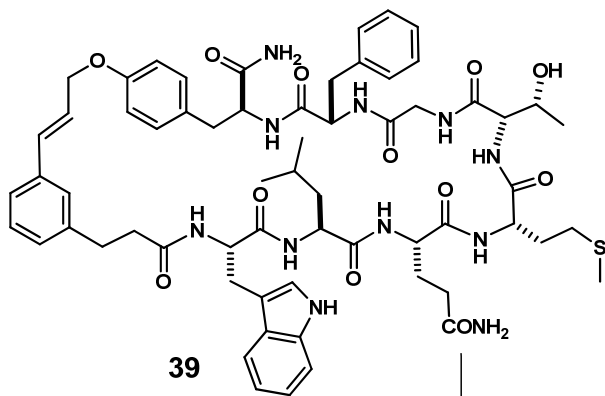


Current Data Parameters
 NAME KL-4-44
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111006
 Time 20.16
 INSTRUM av600
 PROBHD 5 mm TBI5
 PULPROG hsqcetgpsisp
 TD 2048
 SOLVENT DMSO
 NS 48
 DS 16
 SWH 5387.931 H:
 FIDRES 2.630826 H:
 AQ 0.1900544 s:
 RG 26008
 DW 92.800 u:
 DE 6.00 u:
 TE 296.9 K
 CNST2 145.000000
 d0 0.00000300 s:
 D1 1.20000005 s:
 d4 0.00172414 s:
 d11 0.03000000 s:
 D16 0.00020000 s:
 D24 0.00086200 s:
 DELTA 0.00127580 s:
 DELTA1 0.00120628 s:
 DELTA2 0.00097414 s:
 in0 0 sec
 ST1CNT 128
 ZGPTNS
 d0orig 0.00000300 s:
 philloop 0
 t1loop 0
 SFO1 600.1327006 MHz
 NUC1 1H
 P1 9.90 u:
 p2 19.80 u:
 P28 1000.00 u:
 PLW1 -1.00000000 W
 SFO2 150.9133722 MHz
 NUC2 13C
 CPDPRG[2] garp



Cyclic-Trp-Leu-Gln-Met-Thr-Gly-Phe-Tyr (39):

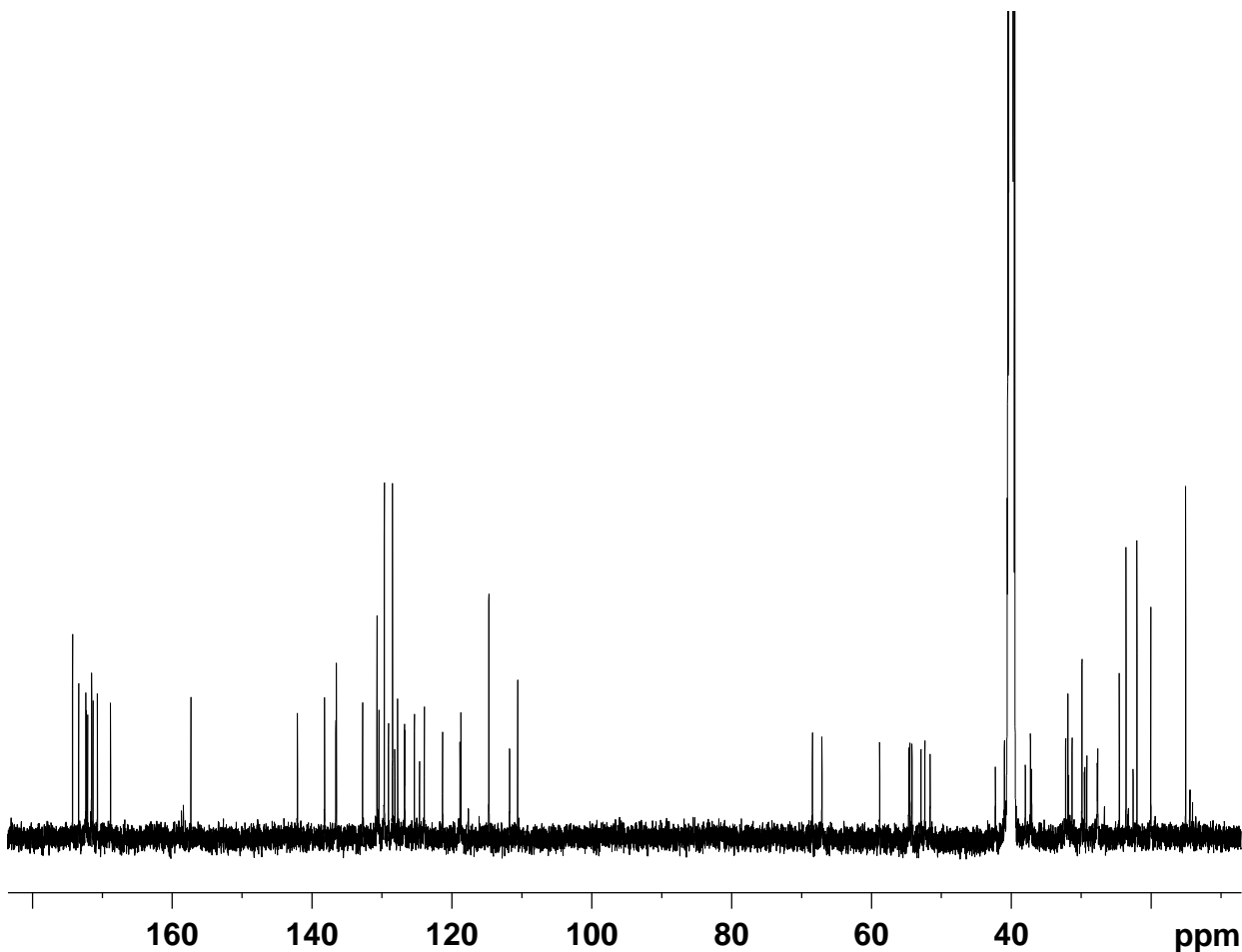


```
Current Data Parameters
NAME      KL-5-124
EXPNO    1
PROCNO    1

F2 - Acquisition Parameters
Date_    20130201
Time     11.51
INSTRUM  av500
PROBHD   5 mm DCH 13C-1
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        8
DS        0
SWH       10000.000 Hz
FIDRES    0.152588 Hz
AQ        3.2767999 sec
RG        22.82
DW        50.000 usec
DE        10.00 usec
TE        298.0 K
D1        2.00000000 sec
D10       1
TD0       1
```

```
===== CHANNEL f1 =====
SFO1     500.1330008 MHz
NUC1      1H
P1        10.00 usec
PLW1     13.50000000 W
```

```
F2 - Processing parameters
SI        65536
SF        500.1300146 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```



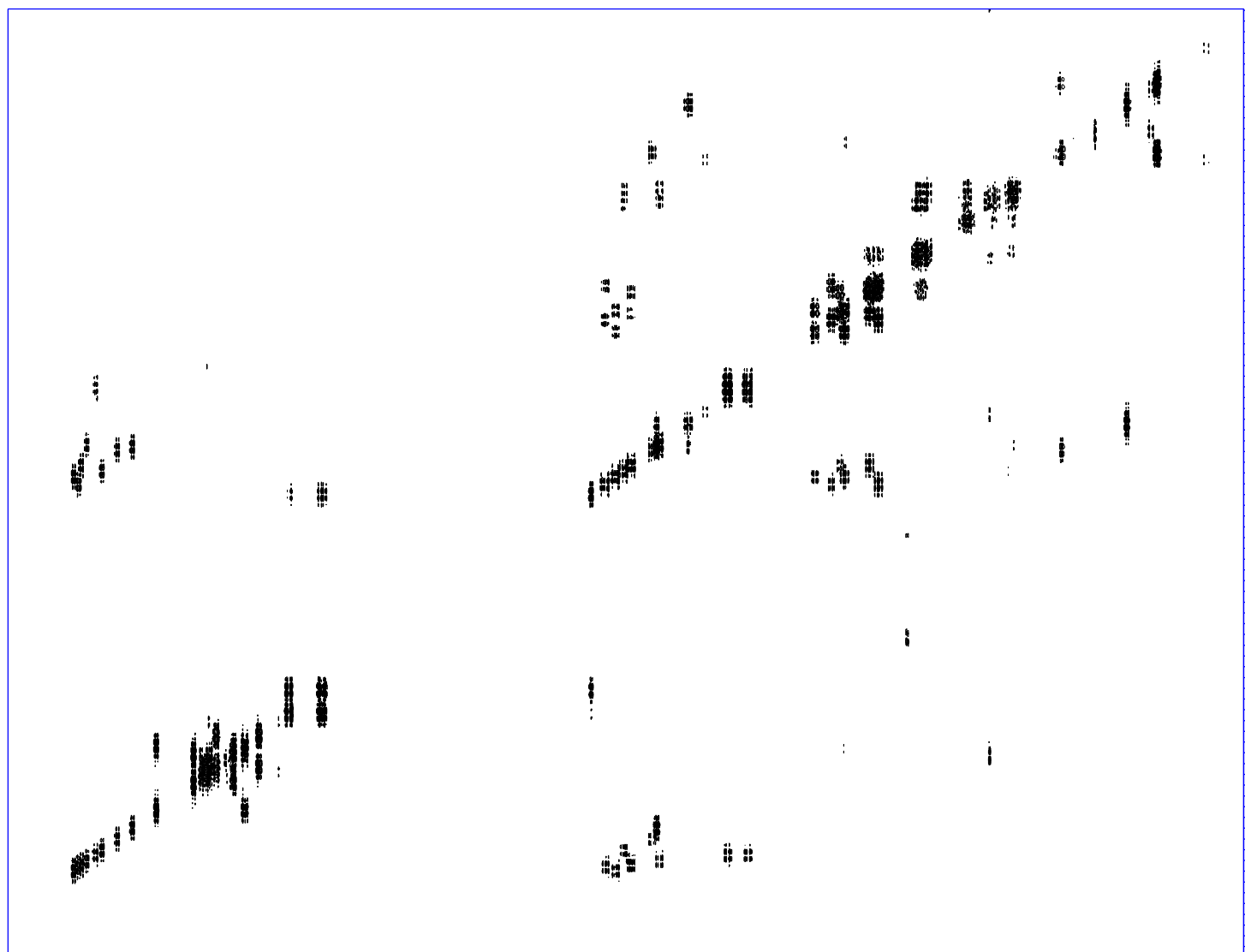
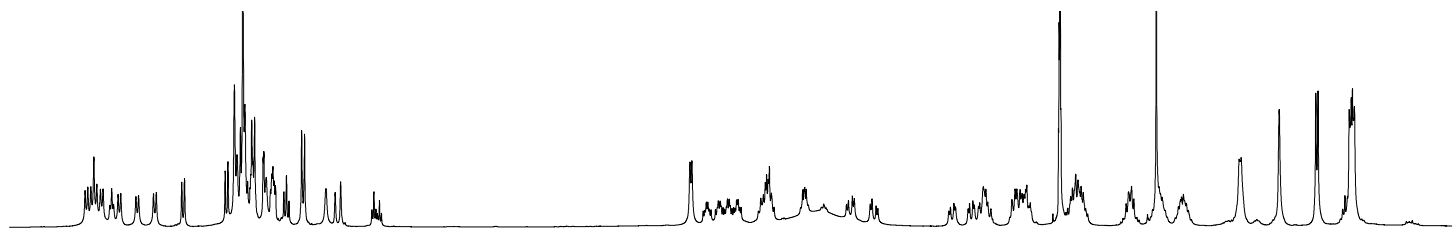
```
Current Data Parameters
NAME      KL-5-124
EXPNO    2
PROCNO    1

F2 - Acquisition Parameters
Date_    20130201
Time     11.53
INSTRUM  av500
PROBHD   5 mm DCH 13C-1
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        162
DS        2
SWH       31250.000 Hz
FIDRES    0.476837 Hz
AQ        1.0485760 sec
RG        202.91
DW        16.000 usec
DE        18.00 usec
TE        298.0 K
D1        2.00000000 sec
D11       0.03000000 sec
D10       1
TD0       1
```

```
===== CHANNEL f1 =====
SFO1     125.7722511 MHz
NUC1      13C
P1        9.63 usec
PLW1     23.00000000 W
```

```
===== CHANNEL f2 =====
SFO2     500.1330008 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     80.00 usec
PLW2     13.50000000 W
PLW12    0.21094000 W
PLW13    0.13500001 W
```

```
F2 - Processing parameters
SI        131072
SF        125.7577892 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```



ppm

0

1

2

3

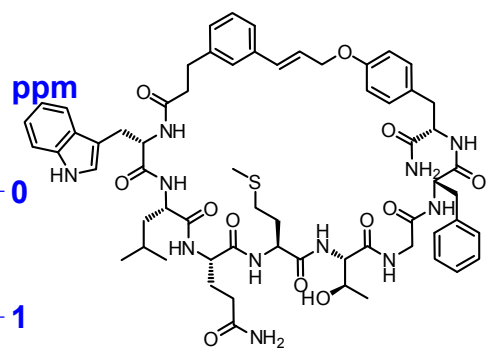
4

5

6

7

8



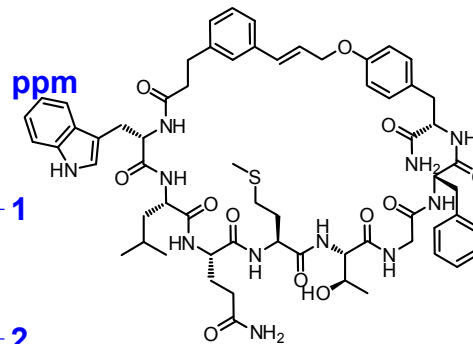
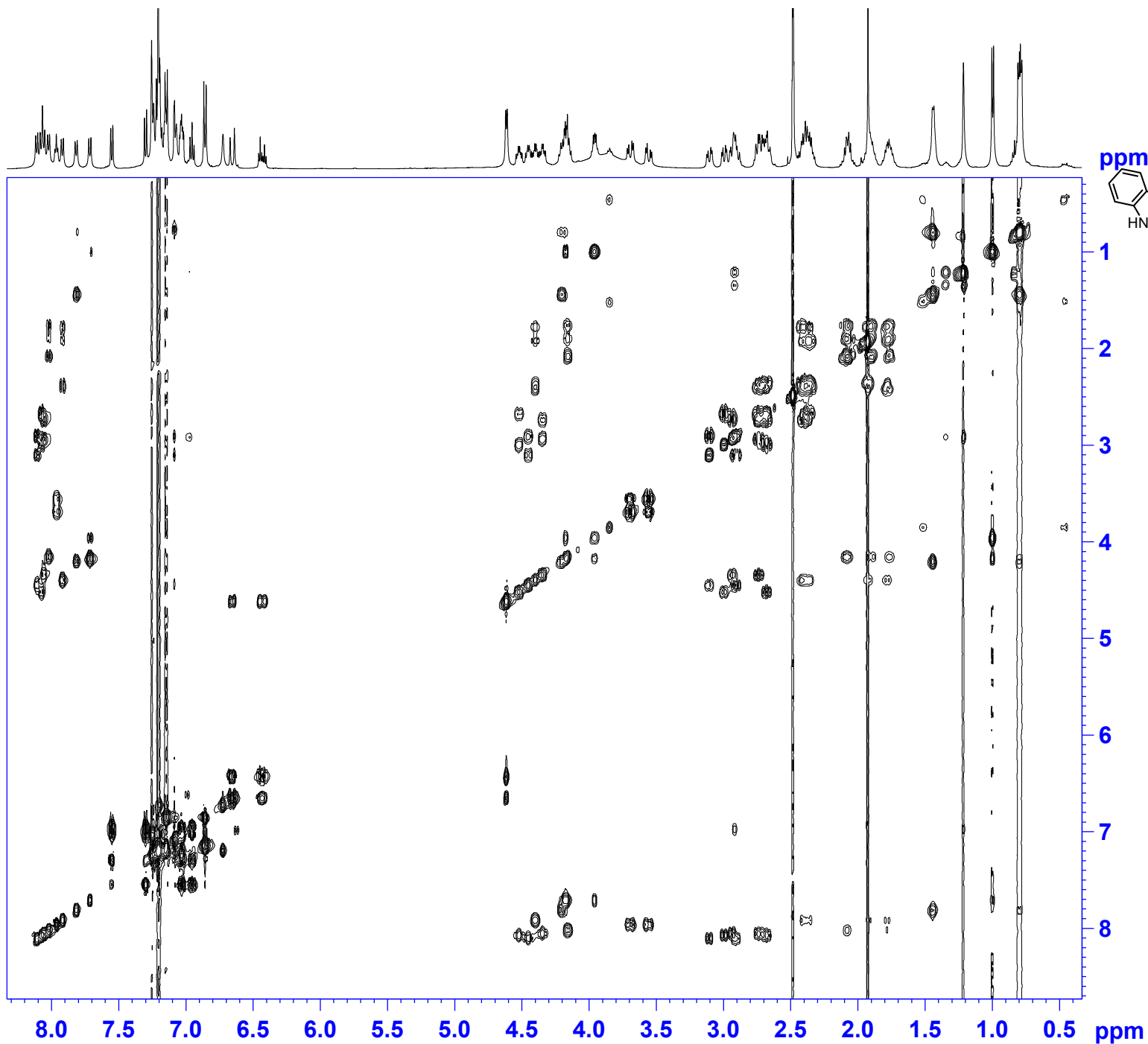
Current Data Parameters
 NAME KL-5-124
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20130204
 Time 19.05
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG cosygmfph
 TD 4096
 SOLVENT DMSO
 NS 2
 DS 8
 SWH 5498.534 H:
 FIDRES 1.342415 H:
 AQ 0.3724629 s:
 RG 202.91
 DW 90.933 u:
 DE 10.00 u:
 TE 298.0 K
 D0 0.00007880 s:
 D1 2.00000000 s:
 D13 0.00000400 s:
 D16 0.00020000 s:
 IN0 0.00018180 s:

==== CHANNEL f1 =====
 SFO1 500.1327507 M:
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 PLW1 13.50000000 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPZ1 10.00 %
 GPZ2 20.00 %
 P16 1000.00 u:

F1 - Acquisition parameters:
 TD 256
 SFO1 500.1328 M:
 FIDRES 21.486525 H:
 SW 10.998 p:

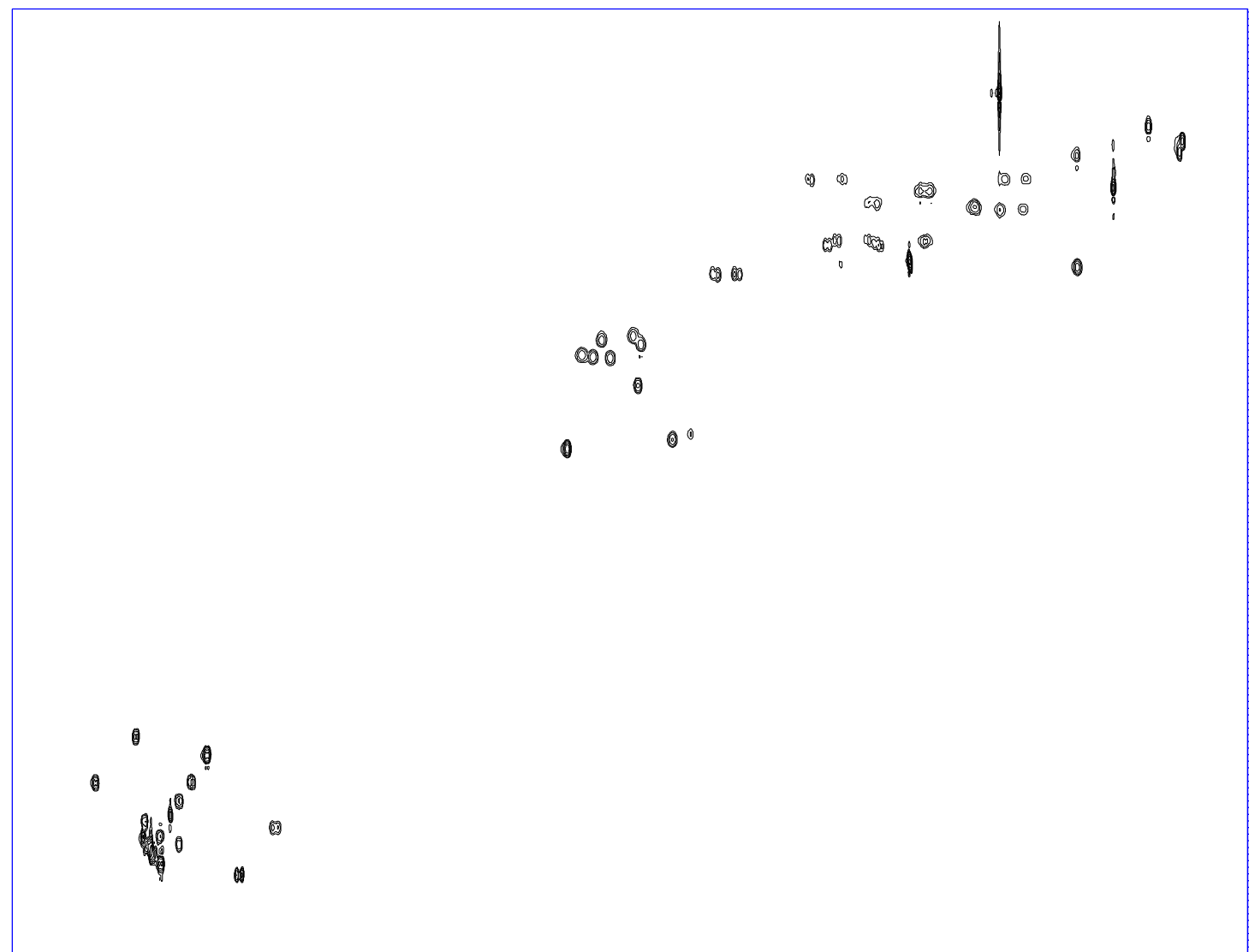
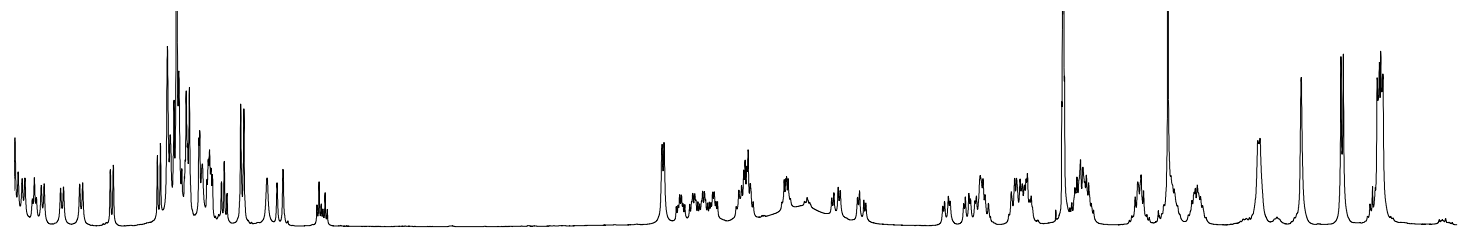


Current Data Parameters
 NAME KL-5-124
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20130204
 Time 19.26
 INSTRUM av500
 PROBHD 5 mm DCH 13C-1
 PULPROG mlevetgp.js
 TD 2048
 SOLVENT DMSO
 NS 2
 DS 8
 SWH 5000.000 H:
 FIDRES 2.441406 H:
 AQ 0.2048000 s:
 RG 37.94
 DW 100.000 u:
 DE 10.00 u:
 TE 298.0 K
 D0 0.00000300 s:
 D1 2.00000000 s:
 D9 0.06000000 s:
 D11 0.03000000 s:
 D12 0.00002000 s:
 D16 0.00020000 s:
 IN0 0.00020000 s:
 L1 24

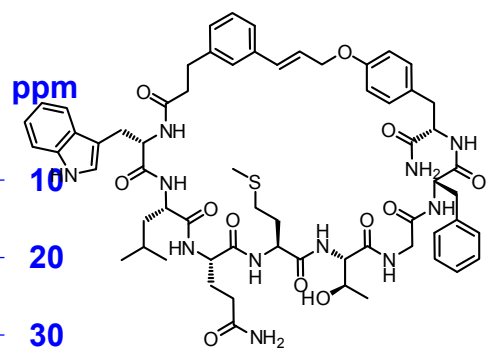
===== CHANNEL f1 =====
 SFO1 500.1325007 MHz
 NUC1 1H
 P1 9.50 u:
 P2 19.00 u:
 P5 26.68 u:
 P6 40.00 u:
 P7 80.00 u:
 P17 2500.00 u:
 PLW1 13.5000000 W
 PLW10 0.84375000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SINE.100
 GPNAM[2] SINE.100
 GPZ1 30.00 %



7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
ppm



Current Data Parameters
NAME KL-5-124
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters:
Date_ 20130204
Time 19.46
INSTRUM av500
PROBHD 5 mm DCH 13C-1
PULPROG hsqcedetgp
TD 2048
SOLVENT DMSO
NS 2
DS 16
SWH 5000.000 H:
FIDRES 2.441406 H:
AQ 0.2048000 s:
RG 202.91
DW 100.000 u:
DE 10.00 u:
TE 298.0 K
CNST2 145.000000
D0 0.00000300 s:
D1 1.50000000 s:
D4 0.00172414 s:
D11 0.03000000 s:
D13 0.00000400 s:
D16 0.00020000 s:
D21 0.00345000 s:
IN0 0.00001990 s:
ZGPTNS

==== CHANNEL f1 =====
SFO1 500.1325007 MHz
NUC1 1H
P1 9.50 u:
P2 19.00 u:
P28 0 usec
PLW1 13.50000000 W

==== CHANNEL f2 =====
SFO2 125.7678496 MHz
NUC2 13C
CPDPRG[2] garp
P3 9.63 u:
P4 19.26 u:

Compound 39

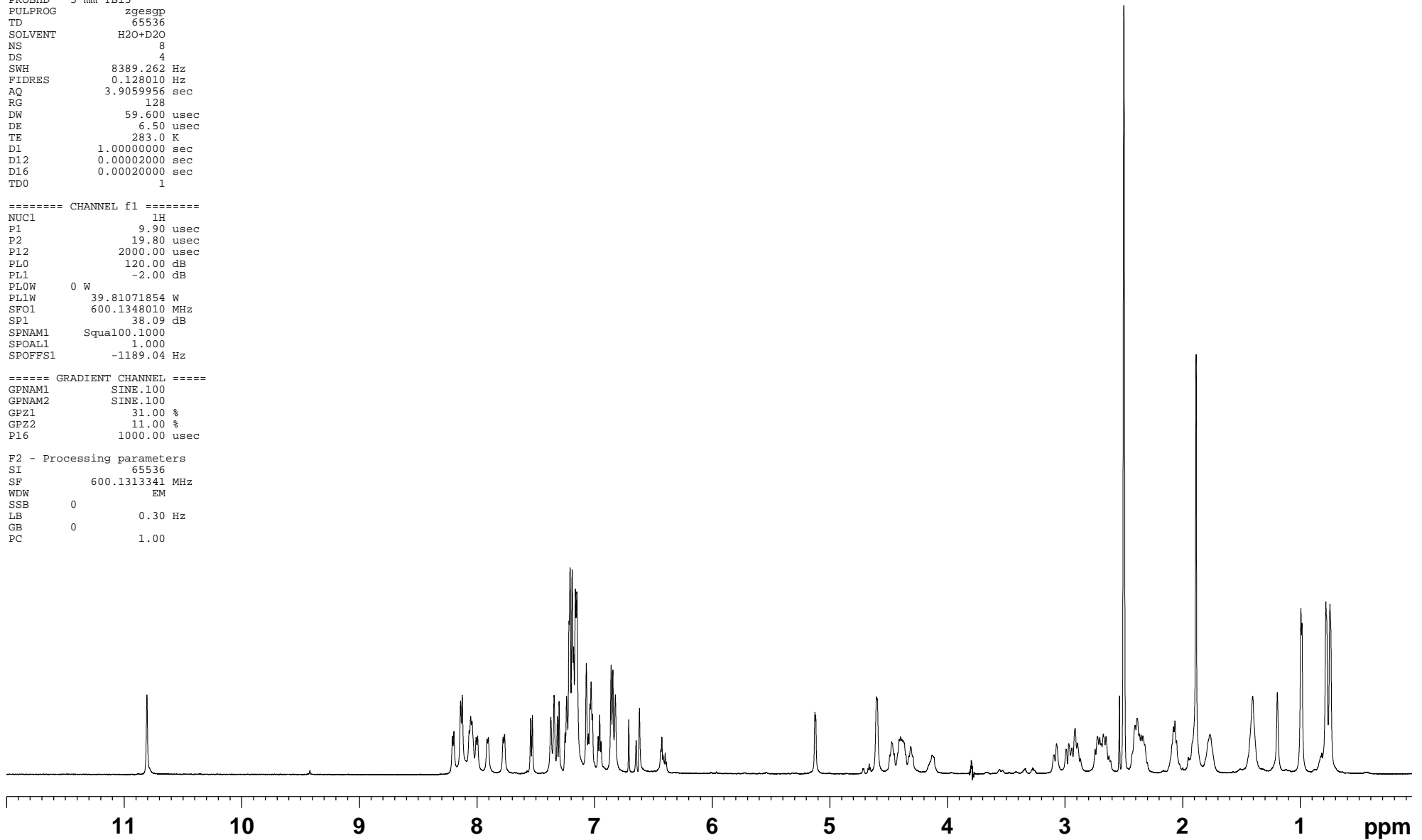
Current Data Parameters
NAME KL5-124
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130314
Time 21.43
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG zgesgp
TD 65536
SOLVENT H2O+D2O
NS 8
DS 4
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 283.0 K
D1 1.00000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
P2 19.80 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -2.00 dB
PLOW 0 W
PL1W 39.81071854 W
SFO1 600.1348010 MHz
SP1 38.09 dB
SPNAM1 Squal00.1000
SPOAL1 1.000
SPOFFS1 -1189.04 Hz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 31.00 %
GPZ2 11.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 600.1313341 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Compound 39

Current Data Parameters
NAME KL5-124 mulder
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130322
Time 13.29
INSTRUM spect
PROBHD 5 mm QXI 1H Z-
PULPROG ecos3cph
TD 2048
SOLVENT D2O
NS 12
DS 32
SWH 2540.650 Hz
FIDRES 1.240552 Hz
AQ 0.4030964 sec
RG 256
DW 196.800 usec
DE 6.00 usec
TE 300.0 K
d0 0.00018381 sec
d1 2.00000000 sec
d13 0.00000400 sec
IN0 0.00039360 sec
MCREST 0 sec
MCWRK 1.00000000 sec
ST1CNT 0

ppm

1

2

3

4

5

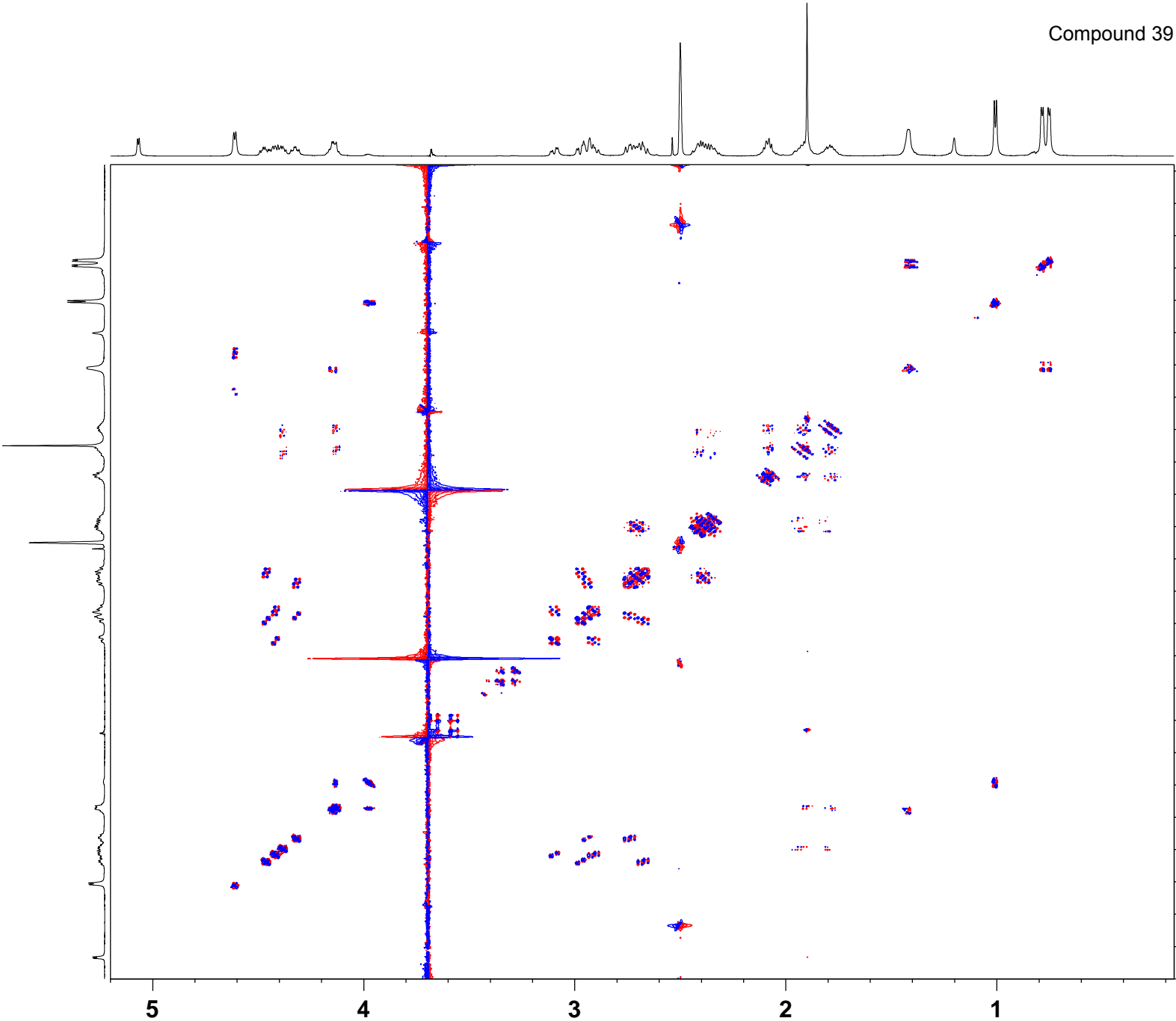
==== CHANNEL f1 =====
NUC1 1H
P1 10.20 usec
PL1 -3.00 dB
SFO1 500.0913502 MHz

F1 - Acquisition parameters
TD 900
SFO1 500.0914 MHz
FIDRES 2.822945 Hz
SW 5.080 ppm
FnMODE States-TPPI

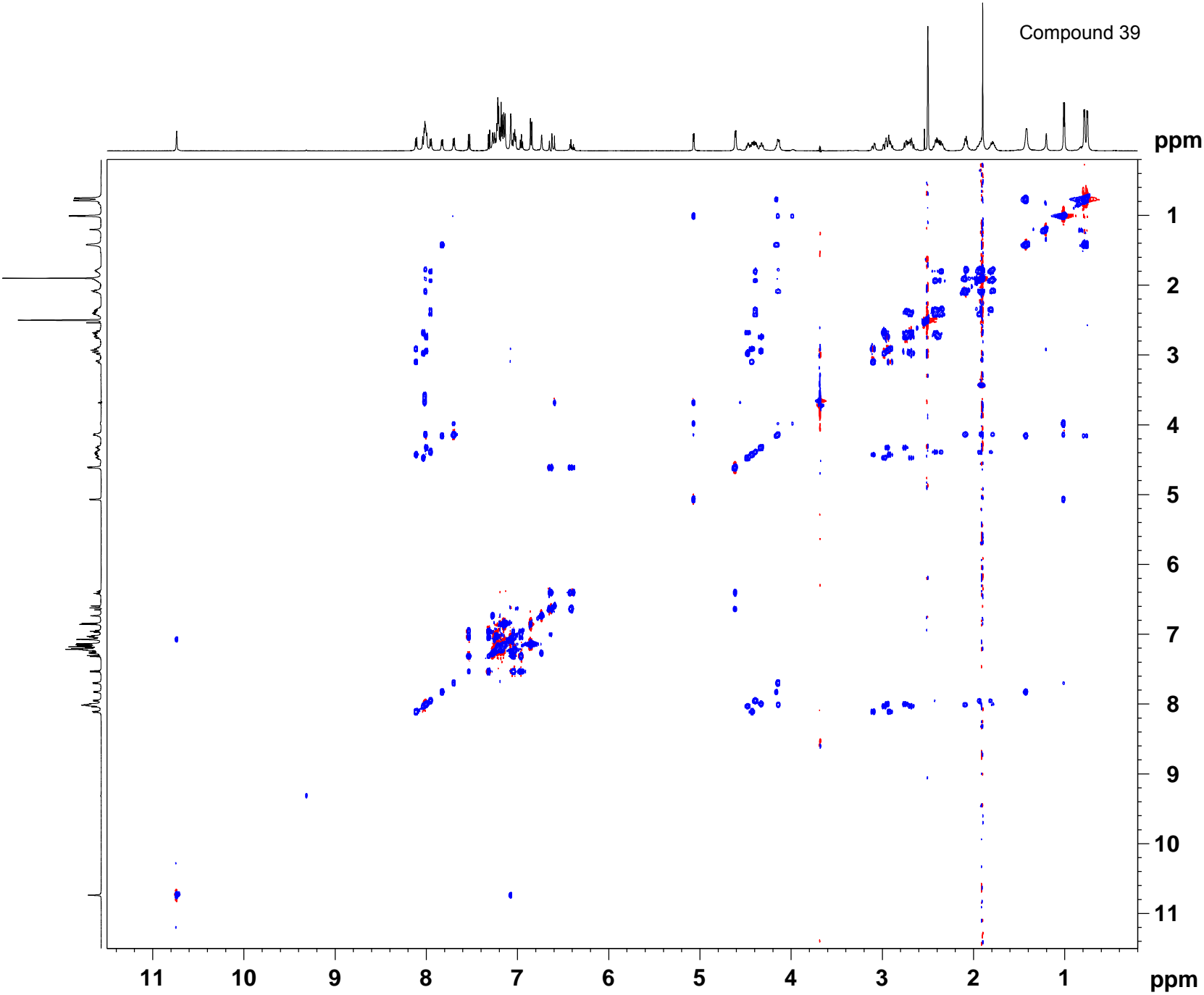
F2 - Processing parameters
SI 4096
SF 500.0900073 MHz
WDW QSINE
SSB 3
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 4096
MC2 States-TPPI
SF 500.0900024 MHz
WDW
SSB 3
LB 0 Hz
GB 0

ppm



Compound 39



```

Current Data Parameters
NAME      KL5-124
EXPNO    13
PROCNO    1

F2 - Acquisition Parameters
Date_     20130312
Time      19.49
INSTRUM   av600
PROBHD    5 mm TBI5
PULPROG   dipsi2esgpph
TD        2048
SOLVENT   H2O+D2O
NS        8
DS        16
SWH       8389.262 Hz
FIDRES    4.096319 Hz
AQ        0.1221108 sec
RG        25.4
DW        59.600 usec
DE        6.50 usec
TE        298.0 K
D0        0.00004687 sec
D1        1.50000000 sec
D9        0.06000000 sec
D11       0.03000000 sec
D12       0.00002000 sec
D13       0.00000400 sec
D16       0.00020000 sec
IN0       0.00011920 sec
L1        14

===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
P2        20.00 usec
P6        40.00 usec
P12       2000.00 usec
PL0       120.00 dB
PL1       -2.00 dB
PL9       80.00 dB
PL10      10.04 dB
PL1W      39.81071854 W
PL9W      0.00000025 W
PL10W     2.48885727 W
SFO1      600.1348010 MHz
SP1       38.00 dB
SPNAM1    Squal00.1000
SPOAL1    1.000
SPOFFS1   -1257.00 Hz

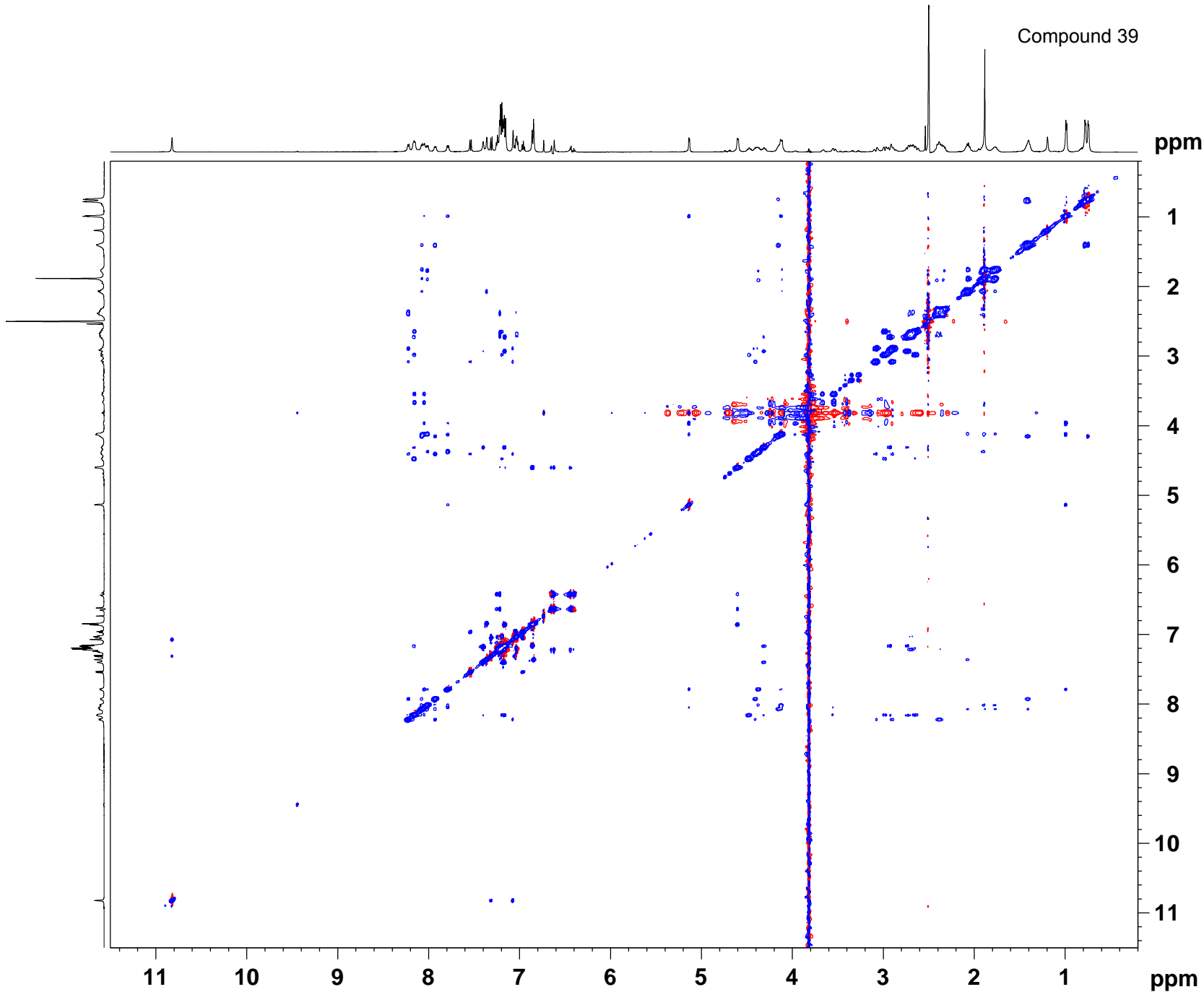
===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPNAM3    SINE.100
GPNAM4    SINE.100
GPZ1      1.00 %
GPZ2      3.00 %
GPZ3      31.00 %
GPZ4      11.00 %
P16       1000.00 usec

F1 - Acquisition parameters
TD        248
SFO1      600.1348 MHz
FIDRES    33.827667 Hz
SW        13.979 ppm
FMODE     States-TPPI

F2 - Processing parameters
SI        4096
SF        600.1313340 MHz
WDW       QSINE
SSB       2.5
PC        1.00

F1 - Processing parameters
SI        4096
MC2       States-TPPI
SF        600.1313332 MHz
WDW       QSINE
SSB       2.5
    
```


Compound 39



```

Current Data Parameters
NAME      KL5-124
EXPNO    47
PROCNO    1

F2 - Acquisition Parameters
Date_     20130316
Time      22.44
INSTRUM   av600
PROBHD    5 mm TBI5
PULPROG   noesyegpph
TD         4096
SOLVENT   H2O+D2O
NS         24
DS         16
SWH        8389.262 Hz
FIDRES     2.048160 Hz
AQ         0.2441716 sec
RG         322.5
DW         59.600 usec
DE         6.50 usec
TE         280.0 K
D0         0.00004657 sec
D1         2.00000000 sec
D8         0.15000001 sec
D11        0.03000000 sec
D12        0.00002000 sec
D16        0.00020000 sec
IN0        0.00011920 sec

===== CHANNEL f1 =====
NUC1       1H
P1         10.23 usec
P2         20.46 usec
P12        3000.00 usec
PL0        120.00 dB
PL1        -2.00 dB
PL0W       0 W
PL1W       39.81071854 W
SFO1       600.1348010 MHz
SP1        43.82 dB
SPNAM1     Squa100.1000
SPOAL1     1.000
SPOFFS1    -1176.04 Hz

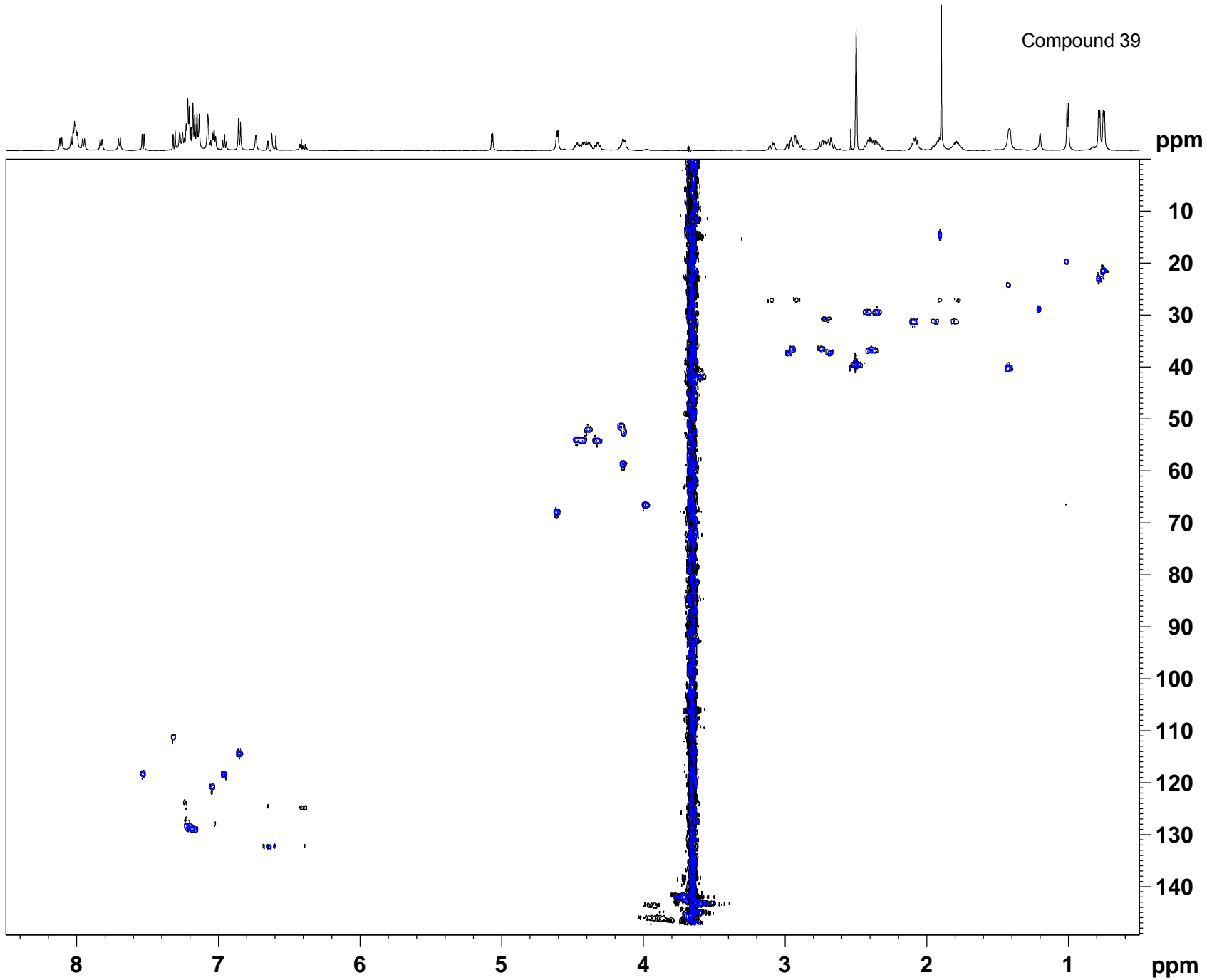
===== GRADIENT CHANNEL =====
GPNAM1     SINE.100
GPNAM2     SINE.100
GPZ1       31.00 %
GPZ2       11.00 %
P16        1000.00 usec

F1 - Acquisition parameters
TD         512
SFO1       600.1348 MHz
FIDRES     16.385277 Hz
SW         13.979 ppm
FnMODE     States-TPPI

F2 - Processing parameters
SI         4096
SF         600.1313334 MHz
WDW        QSINE
SSB        2.5
LB         0 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         4096
MC2        States-TPPI
SF         600.1313325 MHz
WDW        QSINE
SSB        2.5
LB         0 Hz
GB         0
    
```

Compound 39



Current Data Parameters
NAME KL5-124
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130314
Time 18.55
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG hsqcetgpgsisp
TD 2048
SOLVENT H2O+D2O
NS 8
DS 16
SWH 5165.289 Hz
FIDRES 2.522114 Hz
AQ 0.1982964 sec
RG 2608
DW 96.800 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
D0 0.0000300 sec
D1 1.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086200 sec
IN0 0.00002070 sec
ZGOPTNS

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
P2 19.80 usec
P28 1000.00 usec
PL1 -2.00 dB
PL1W 39.81071854 W
SFO1 600.1339609 MHz

==== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 19.52 usec
P4 39.04 usec
P14 1000.00 usec
PCPD2 65.00 usec
PL0 120.00 dB
PL2 -3.00 dB
PL12 7.45 dB
PL2W 150.35617065 W
PL12W 13.55567932 W
SFO2 150.9133722 MHz
SP3 4.12 dB
SPNAM3 Crp80,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz

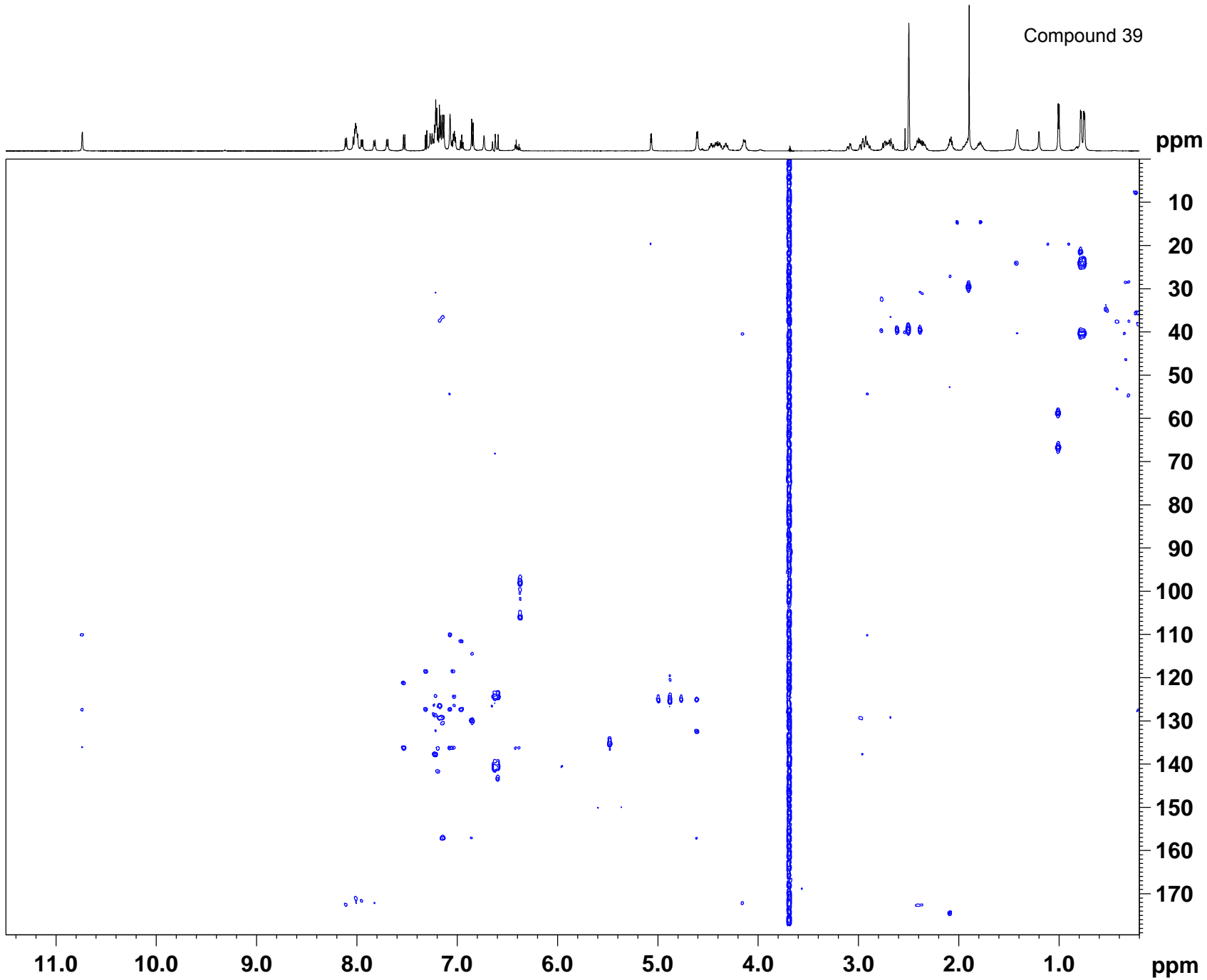
==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 169
SFO1 150.9134 MHz
FIDRES 142.876572 Hz
SW 160.000 ppm
FrnMODE Echo-Antiecho

F2 - Processing parameters
SI 4096
SF 600.1313329 MHz
WDW EM
SSB 0
LB 1.00 Hz
PC 1.40

F1 - Processing parameters
SI 4096
MC2 echo-antiecho
SF 150.9032019 MHz
WDW SINE
SSB 2.5

Compound 39



Current Data Parameters
NAME KL5-124
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130314
Time 19.37
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG hmcgplndqf
TD 2048
SOLVENT H2O+D2O
NS 24
DS 64
SWH 6887.052 Hz
FIDRES 3.362818 Hz
AQ 0.1487348 sec
RG 26008
DW 72.600 usec
DE 6.00 usec
TE 298.0 K
CNST2 145.0000000
CNST13 7.0000000
D0 0.00000300 sec
D1 1.00000000 sec
D2 0.00344828 sec
D6 0.07142857 sec
D16 0.00020000 sec
INO 0.00001745 sec

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
P2 19.80 usec
PL1 -2.00 dB
PL1W 39.81071854 W
SFO1 600.1347710 MHz

==== CHANNEL f2 =====
NUC2 13C
P3 19.52 usec
PL2 -3.00 dB
PL2W 150.35617065 W
SFO2 150.9156357 MHz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 197
SFO1 150.9156 MHz
FIDRES 145.553146 Hz
SW 190.000 ppm
FnMODE QF

F2 - Processing parameters
SI 4096
SF 600.1313342 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 QF
SF 150.9031854 MHz
WDW
SSB 2

Compound S33

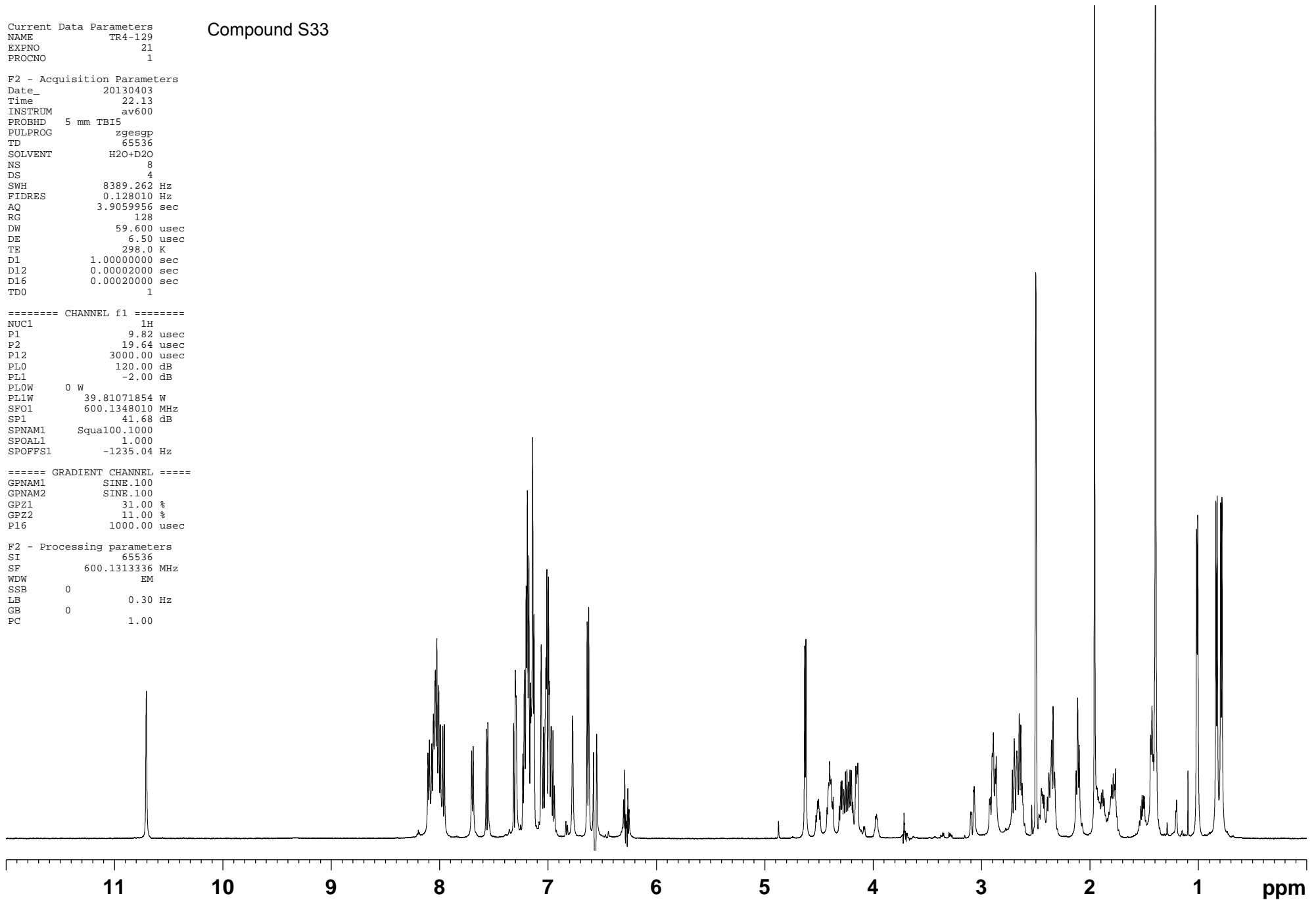
Current Data Parameters
NAME TR4-129
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130403
Time 22.13
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG zgesgp
TD 65536
SOLVENT H2O+D2O
NS 8
DS 4
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.82 usec
P2 19.64 usec
P12 3000.00 usec
PL0 120.00 dB
PL1 -2.00 dB
PLOW 0 W
PL1W 39.81071854 W
SFO1 600.1348010 MHz
SP1 41.68 dB
SPNAM1 Squal00.1000
SPOAL1 1.000
SPOFFS1 -1235.04 Hz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 31.00 %
GPZ2 11.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 600.1313336 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Compound S33

```
Current Data Parameters
NAME TR4-129
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130326
Time 22.05
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG mlevsgppph
TD 2048
SOLVENT H2O+D2O
NS 2
DS 16
SWH 8389.262 Hz
FIDRES 4.096319 Hz
AQ 0.1221108 sec
RG 362
DW 59.600 usec
DE 6.50 usec
TE 323.0 K
D0 0.00003310 sec
D1 1.00000000 sec
D9 0.06000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
INO 0.00011920 sec
LI 24

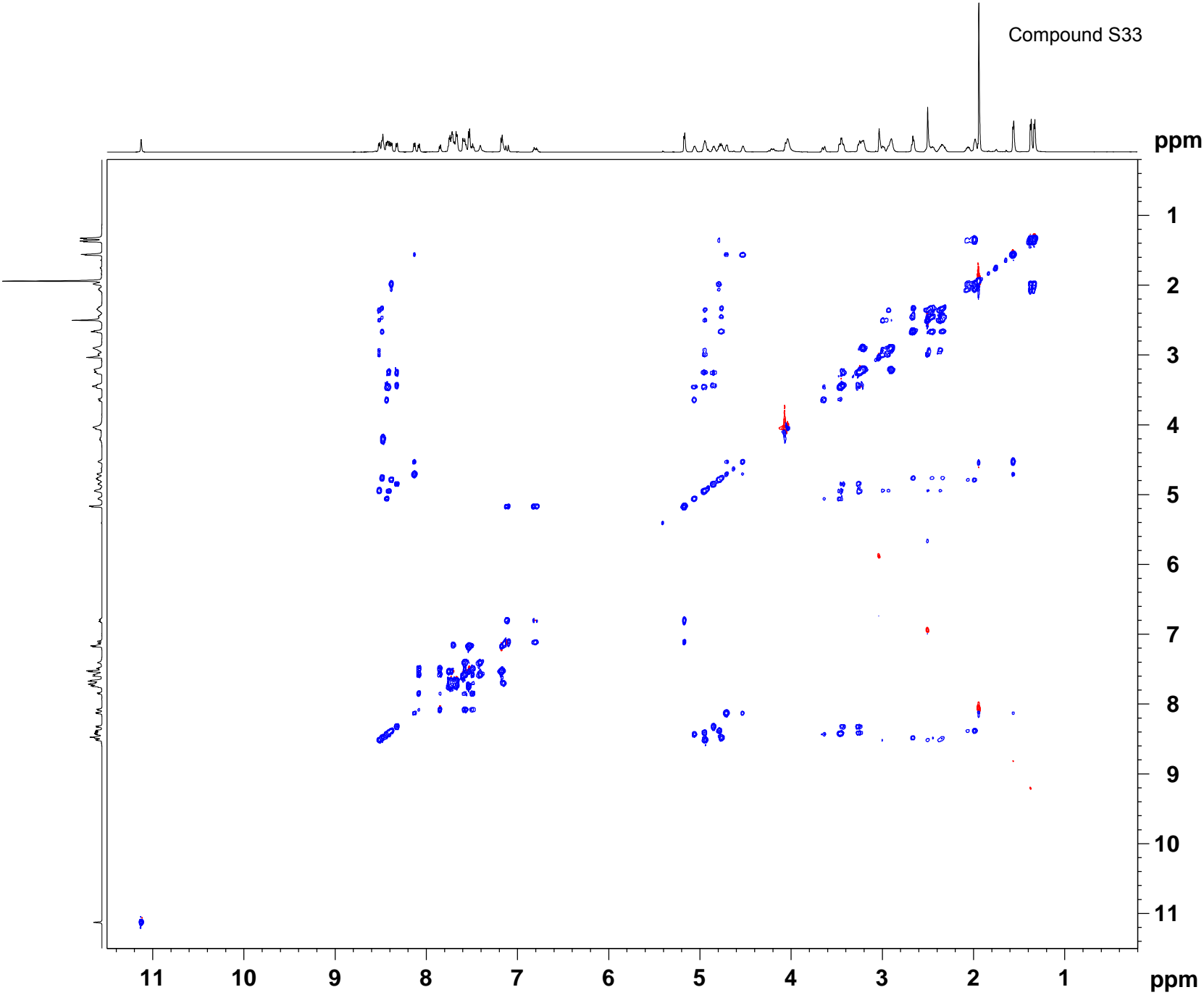
===== CHANNEL f1 =====
NUC1 1H
P1 10.21 usec
P2 20.42 usec
P5 26.68 usec
P6 40.00 usec
P7 80.00 usec
P12 2000.00 usec
P17 2500.00 usec
PL0 120.00 dB
PL1 -2.00 dB
PL10 9.86 dB
PLOW 0 W
PL1W 39.81071854 W
PL10W 2.59417963 W
SF01 600.1348010 MHz
SP1 37.82 dB
SPNAM1 Squa100.1000
SFOALL 1.000
SPOFFS1 -1345.04 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 31.00 %
GPZ2 11.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 600.1348 MHz
FIDRES 32.770554 Hz
SW 13.979 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 4096
SF 600.1310113 MHz
WDW QSINE
SSB 2
PC 1.00

F1 - Processing parameters
SI 4096
MC2 States-TPPI
SF 600.1310119 MHz
WDW
SSB 2
```



Compound S33

Current Data Parameters
NAME TR4-129
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130403
Time 22.20
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG noesyegpph
TD 4096
SOLVENT H2O+D2O
NS 8
DS 16
SWH 8389.262 Hz
FIDRES 2.048160 Hz
AQ 0.2441716 sec
RG 574.7
DW 59.600 usec
DE 6.50 usec
TE 298.0 K
D0 0.00004710 sec
D1 2.00000000 sec
D8 0.30000001 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
INO 0.00011920 sec

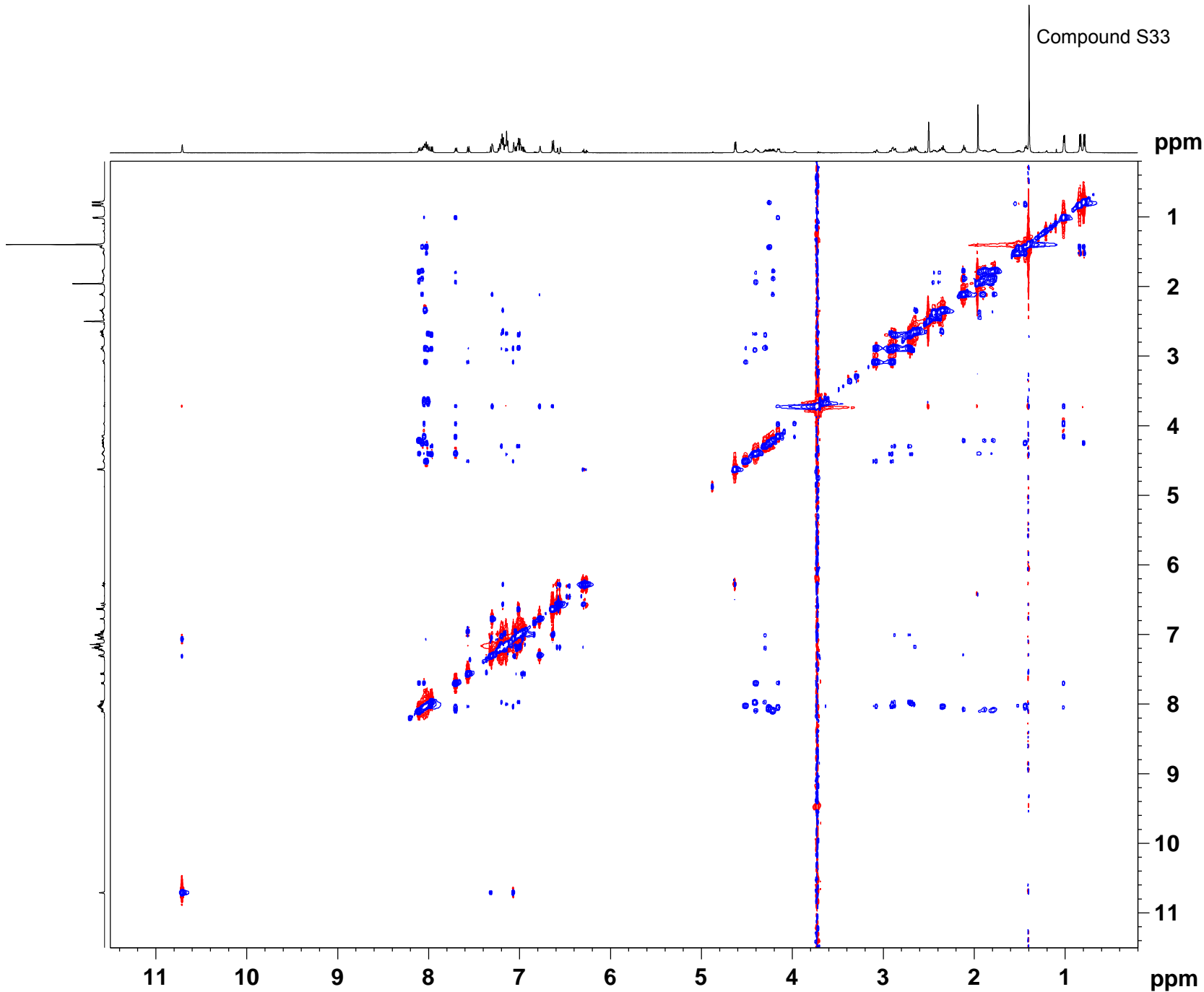
==== CHANNEL f1 =====
NUC1 1H
P1 9.82 usec
P2 19.64 usec
P12 3000.00 usec
PL0 120.00 dB
PL1 -2.00 dB
PLOW 0 W
PLIW 39.81071854 W
SFO1 600.1348010 MHz
SPL 41.68 dB
SPNAM1 Squal00.1000
SPOAL1 1.000
SPOFFS1 -1171.44 Hz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 31.00 %
GPZ2 11.00 %
PI6 1000.00 usec

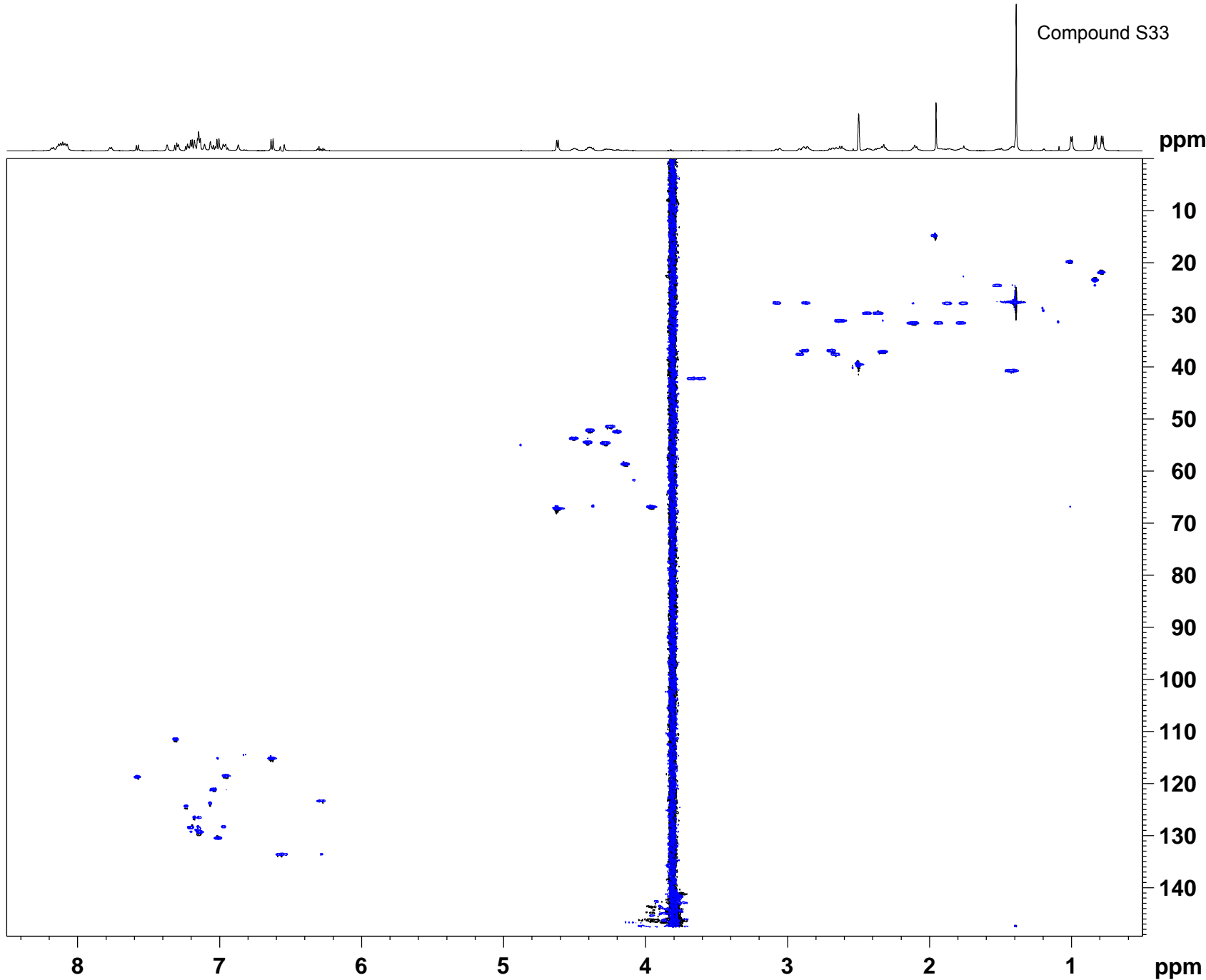
F1 - Acquisition parameters
TD 256
SFO1 600.1348 MHz
FIDRES 32.770527 Hz
SW 13.979 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 4096
SF 600.1313313 MHz
WDW QSINE
SSB 2
PC 1.00

F1 - Processing parameters
SI 4096
MC2 States-TPPI
SF 600.1313330 MHz
WDW
SSB 3



Compound S33



```
Current Data Parameters
NAME          TR4-129
EXPNO         17
PROCNO        1

F2 - Acquisition Parameters
Date_         20130326
Time          23:30
INSTRUM       av600
PROBHD        5 mm TBI5
PULPROG       hsqcztgppisip
TD            2048
SOLVENT       H2O+D2O
NS            4
DS            16
SWH           4921.260 Hz
FIDRES        2.402959 Hz
AQ            0.2081268 sec
RG            8192
DW            101.600 usec
DE            6.00 usec
TE            283.1 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.00000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086200 sec
INO           0.00002070 sec
ZGOPTNS

===== CHANNEL f1 =====
NUC1          1H
P1            9.90 usec
P2            19.80 usec
P28           1000.00 usec
PL1           -2.00 dB
PL1W          39.81071854 W
SFO1          600.1340570 MHz

===== CHANNEL f2 =====
CPDPRG2       garp
NUC2          13C
P3            19.52 usec
P4            39.04 usec
P14           1000.00 usec
PCPD2         65.00 usec
PL0           120.00 dB
PL2           -3.00 dB
PL12          7.45 dB
PL0W          0 W
PL2W          150.35617065 W
PL12W         13.55567932 W
SFO2          150.9133722 MHz
SP3           4.12 dB
SPNAM3        Crp80,0.5,20.1
SFOAL3        0.500
SPOFFS3       0 Hz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPZ1          80.00 %
GPZ2          20.10 %
P16           1000.00 usec

F1 - Acquisition parameters
TD            512
SFO1          150.9134 MHz
FIDRES        47.160427 Hz
SW            160.000 ppm
FrnMODE       Echo-Antiecho

F2 - Processing parameters
SI            4096
SF            600.1313271 MHz
WDW           EM
SSB           0
LB            1.00 Hz
PC            1.40

F1 - Processing parameters
SI            4096
MC2           echo-antiecho
SF            150.9031701 MHz
WDW           2.5
SSB           2.5
```

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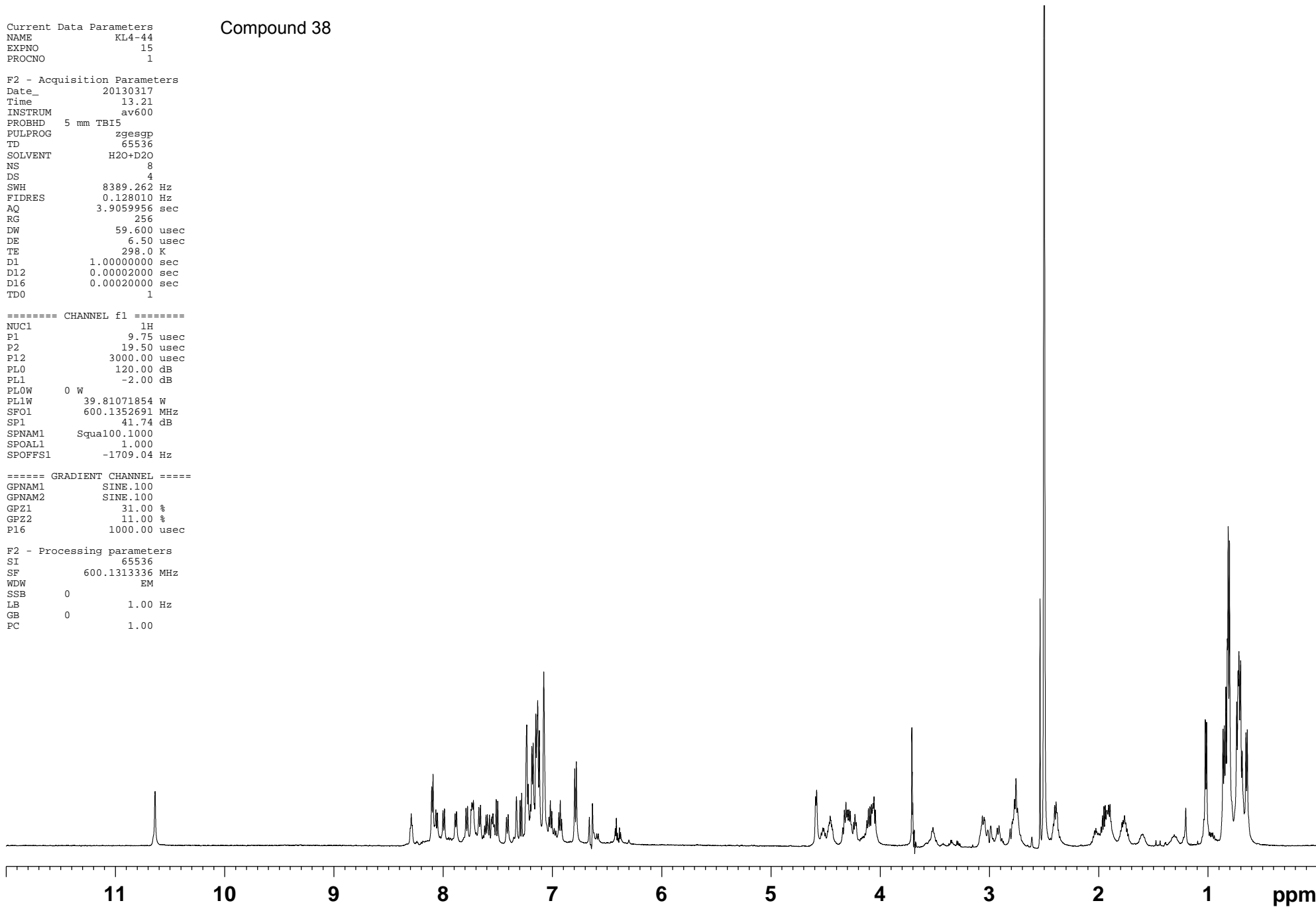
Current Data Parameters
NAME KL4-44
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130317
Time 13.21
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG zgesgp
TD 65536
SOLVENT H2O+D2O
NS 8
DS 4
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 256
DW 59.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

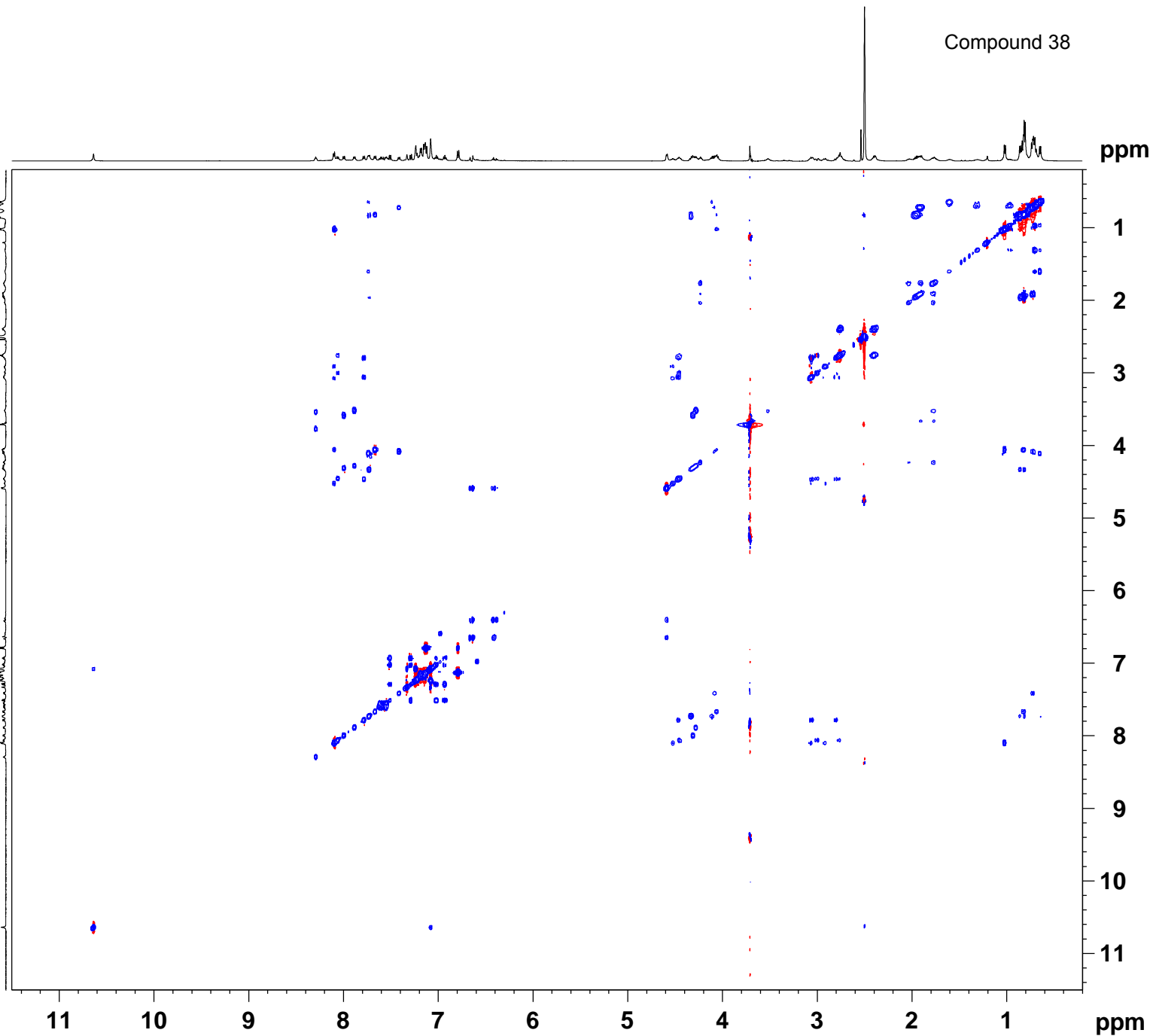
==== CHANNEL f1 =====
NUC1 1H
P1 9.75 usec
P2 19.50 usec
P12 3000.00 usec
PL0 120.00 dB
PL1 -2.00 dB
PLOW 0 W
PLLW 39.81071854 W
SFO1 600.1352691 MHz
SP1 41.74 dB
SPNAM1 Sqa100.1000
SPOAL1 1.000
SPOFFS1 -1709.04 Hz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 31.00 %
GPZ2 11.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 600.1313336 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



Compound 38



Current Data Parameters
 NAME KL4-44
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130316
 Time 20.12
 INSTRUM av600
 PROBHD 5 mm TBI5
 PULPROG dipsi2esgpph
 TD 2048
 SOLVENT H2O+d2o
 NS 8
 DS 16
 SWH 8389.262 Hz
 FIDRES 4.096319 Hz
 AQ 0.1221108 sec
 RG 812.7
 DW 59.600 usec
 DE 6.50 usec
 TE 298.0 K
 D0 0.00004719 sec
 D1 1.00000000 sec
 D9 0.06000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00011920 sec
 L1 14

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.75 usec
 P2 19.50 usec
 P6 40.00 usec
 P12 2000.00 usec
 PL0 120.00 dB
 PL1 -2.00 dB
 PL9 80.00 dB
 PL10 10.26 dB
 PLOW 0 W
 PLLW 39.81071854 W
 PL9W 0.00000025 W
 PL10W 2.36591959 W
 SFO1 600.1352691 MHz
 SF1 38.22 dB
 SPNAM1 Squa100.1000
 SFOAL1 1.000
 SPOFFS1 -1706.14 Hz

==== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPNAM3 SINE.100
 GPNAM4 SINE.100
 GPZ1 1.00 %
 GPZ2 9.00 %
 GPZ3 31.00 %
 GPZ4 11.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 256
 SFO1 600.1353 MHz
 FIDRES 32.770580 Hz
 SW 13.979 ppm
 FMODE States-TPPI

F2 - Processing parameters
 SI 4096
 SF 600.1313331 MHz
 WDW QSINE
 SSB 2
 PC 1.00

F1 - Processing parameters
 SI 4096
 MC2 States-TPPI
 SF 600.1313317 MHz
 WDW
 SSB 3

Compound 38

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Current Data Parameters
NAME          KL4-44
EXPNO         16
PROCNO        1

F2 - Acquisition Parameters
Date_         20130317
Time          13.24
INSTRUM       av600
PROBHD        5 mm TBI5
PULPROG       noesygpph
TD            4096
SOLVENT       H2O+D2O
NS            8
DS            16
SWH           8389.262 Hz
FIDRES        2.048160 Hz
AQ            0.2441716 sec
RG            1625.5
DW            59.600 usec
DE            6.50 usec
TE            298.0 K
D0            0.00004719 sec
D1            2.00000000 sec
D8            0.30000001 sec
D11           0.03000000 sec
D12           0.00020000 sec
D16           0.00020000 sec
IN0           0.00011920 sec

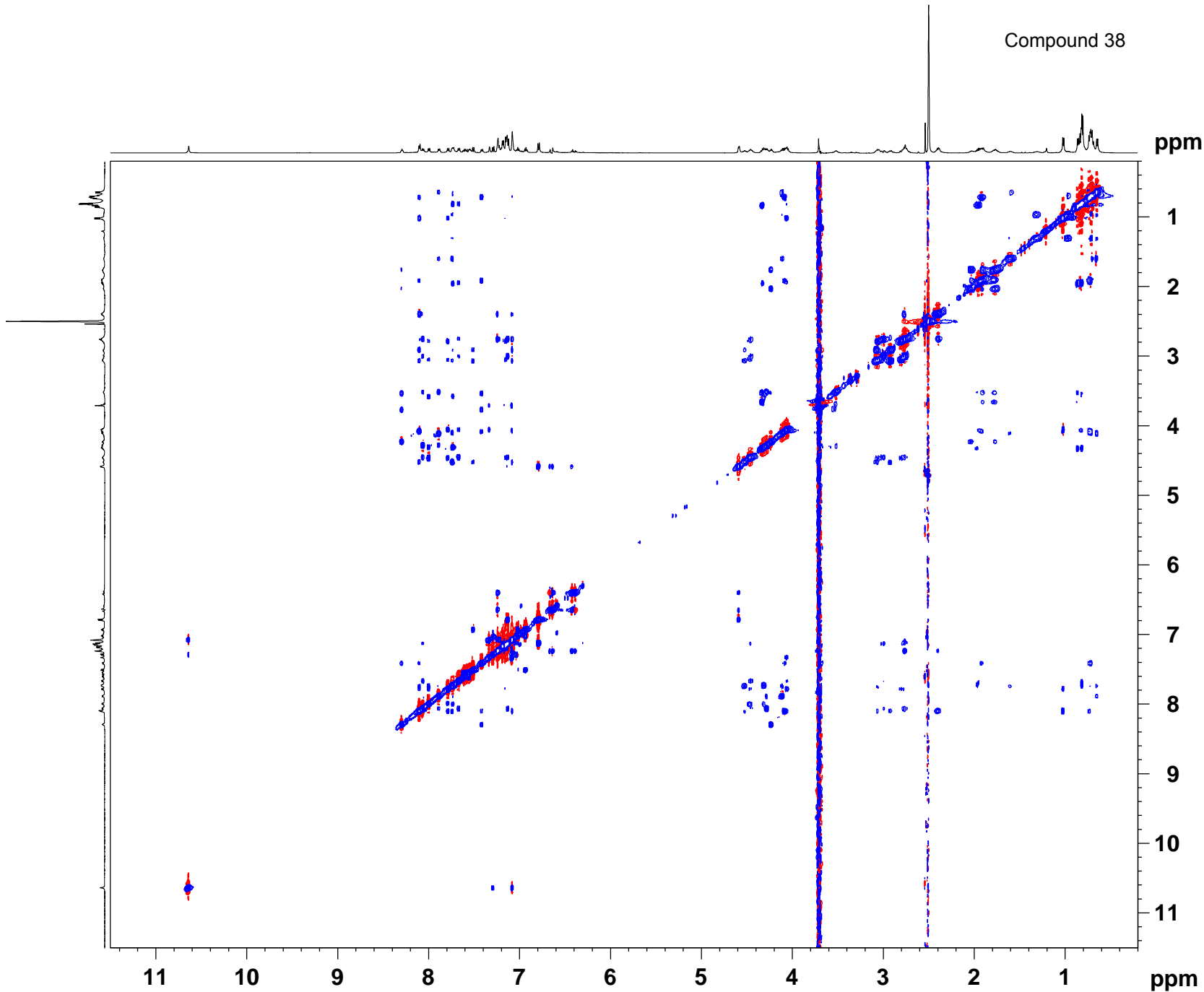
===== CHANNEL f1 =====
NUC1          1H
P1            9.75 usec
P2            19.50 usec
P12           3000.00 usec
PL0           120.00 dB
PL1           -2.00 dB
PL0W          0 W
PL1W          39.81071854 W
SFO1          600.1352691 MHz
SP1           41.74 dB
SFO1          Squal100.1000
SFOAL1        1.000
SFOFFS1       -1710.14 Hz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPZ1          31.00 %
GPZ2          11.00 %
P16           1000.00 usec

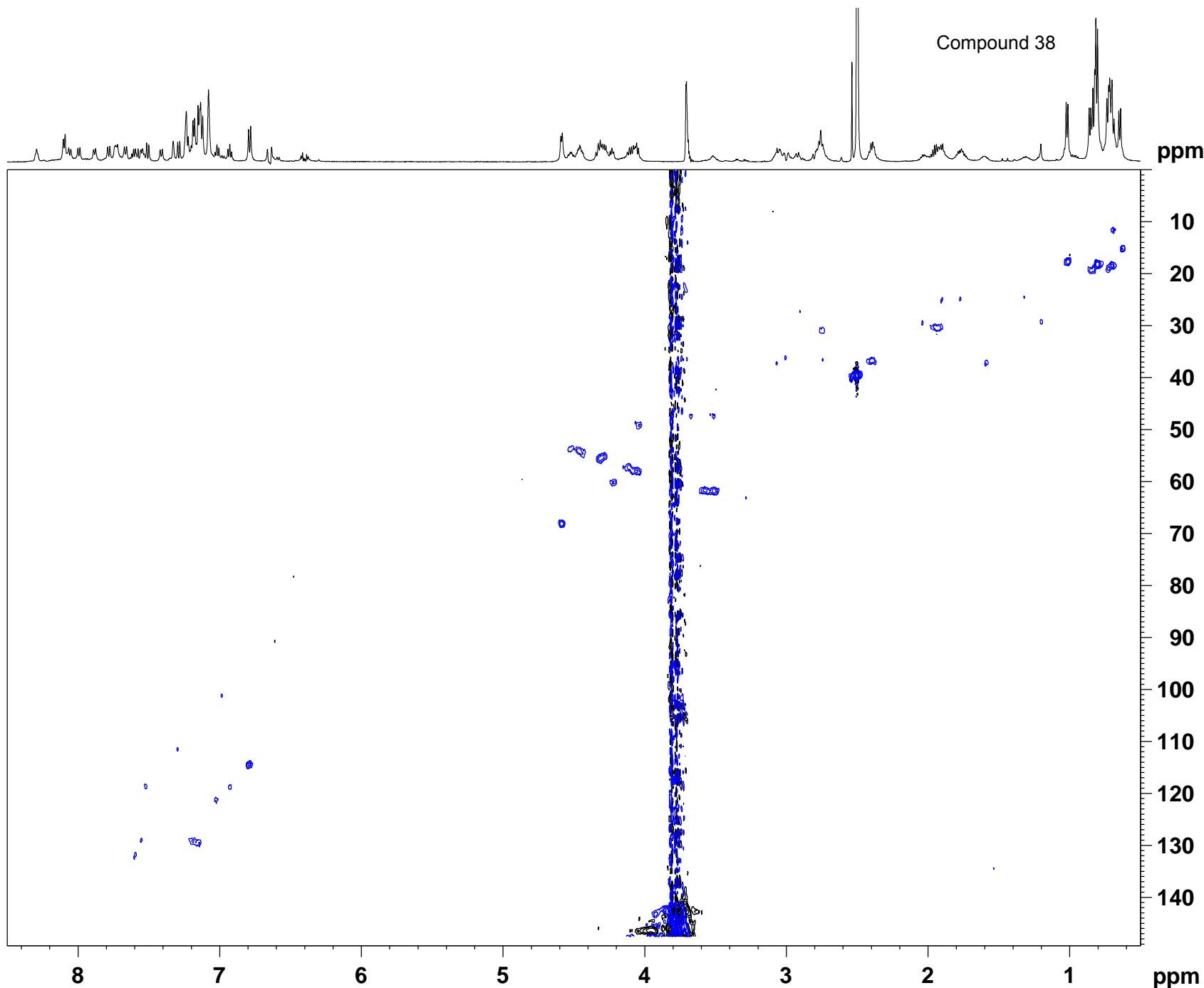
F1 - Acquisition parameters
TD            256
SFO1          600.1353 MHz
FIDRES        32.770554 Hz
SW            13.979 ppm
FnMODE        States-TPPI

F2 - Processing parameters
SI            4096
SF            600.1313328 MHz
WDW           QSINE
SSB           2
PC            1.00

F1 - Processing parameters
SI            4096
MC2           States-TPPI
SF            600.1313335 MHz
WDW           QSINE
SSB           3
    
```



Compound 38



Current Data Parameters
 NAME KL4-44
 EXPNO 18
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130402
 Time 22.01
 INSTRUM av600
 PROBHD 5 mm TBI5
 PULPROG hsqcetgppsisp
 TD 2048
 SOLVENT H2O+D2O
 DS 16
 NS 8
 SWH 4921.260 Hz
 FIDRES 2.402959 Hz
 AQ 0.2081268 sec
 RG 8192
 DW 101.600 usec
 DE 6.00 usec
 TE 283.0 K
 CNST2 145.0000000
 D0 0.00000300 sec
 D1 1.00000000 sec
 D4 0.00172414 sec
 D11 0.03000000 sec
 D16 0.00020000 sec
 D24 0.00086200 sec
 INO 0.00002070 sec
 ZGOPTNS

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.96 usec
 P2 19.92 usec
 P28 1000.00 usec
 PL1 -2.00 dB
 PL1W 39.81071854 W
 SFO1 600.1340570 MHz

==== CHANNEL f2 =====
 CPDPRG2 garp
 NUC2 13C
 P3 19.52 usec
 P4 39.04 usec
 P14 1000.00 usec
 PCPD2 65.00 usec
 PL0 120.00 dB
 PL2 -3.00 dB
 PL12 7.45 dB
 PL0W 0 W
 PL2W 150.35617065 W
 PL12W 13.55567932 W
 SFO2 150.9133722 MHz
 SP3 4.12 dB
 SPNAM3 Crp80,0.5,20.1
 SFOAL3 0.500
 SPOFFS3 0 Hz

==== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPZ1 80.00 %
 GPZ2 20.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 134
 SFO1 150.9134 MHz
 FIDRES 180.195068 Hz
 SW 160.000 ppm
 FmMODE Echo-Antiecho

F2 - Processing parameters
 SI 4096
 SF 600.1313293 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 4096
 MC2 echo-antiecho
 SF 150.9031686 MHz
 WDW
 SSB 2.5
 LB 0 Hz
 GB 0

Current Data Parameters
NAME TR4-133
EXPNO 18
PROCNO 1

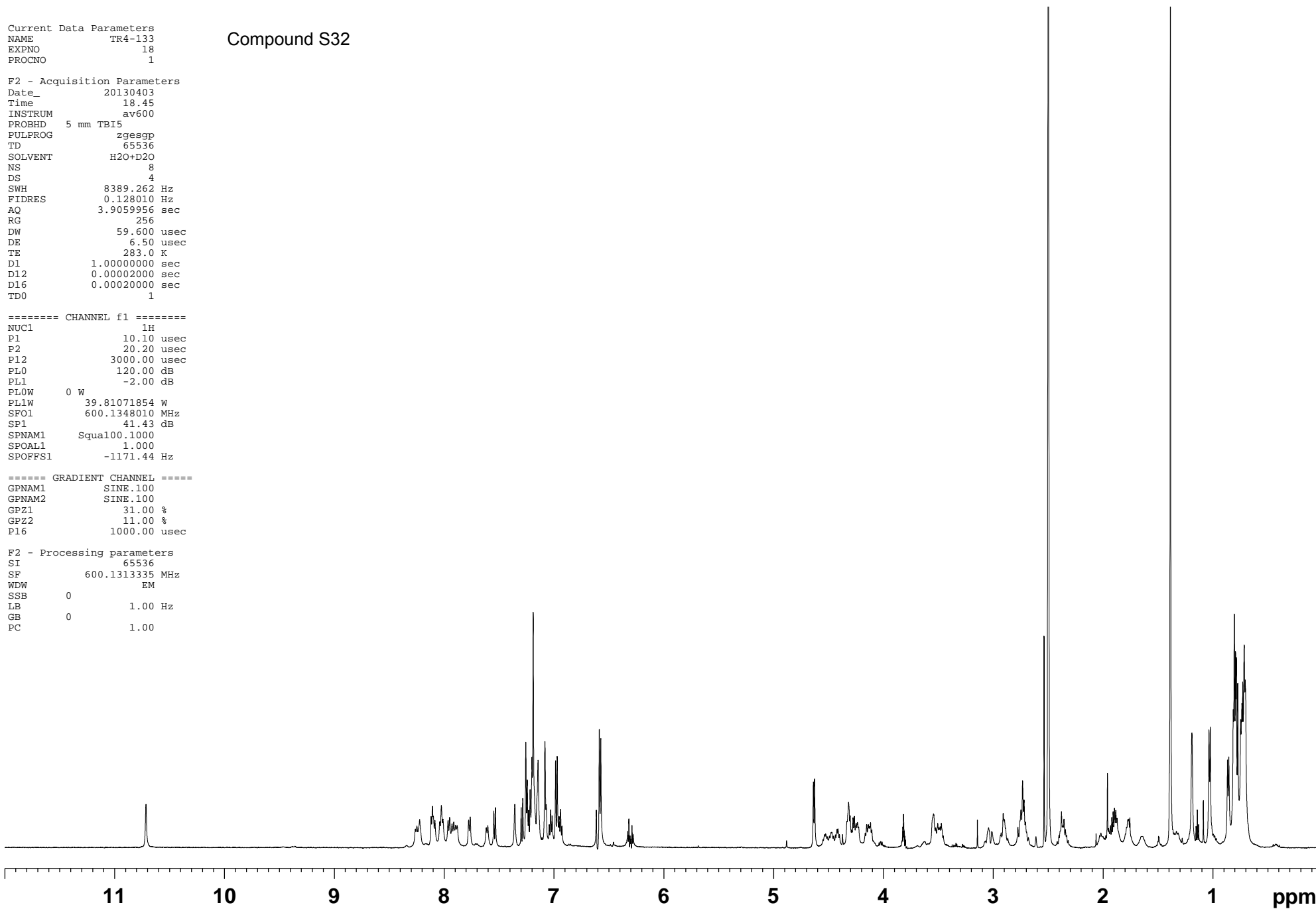
Compound S32

F2 - Acquisition Parameters
Date_ 20130403
Time 18.45
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG zgesgp
TD 65536
SOLVENT H2O+D2O
NS 8
DS 4
SWH 8389.262 Hz
FIDRES 0.128010 Hz
AQ 3.9059956 sec
RG 256
DW 59.600 usec
DE 6.50 usec
TE 283.0 K
D1 1.00000000 sec
D12 0.00020000 sec
D16 0.00020000 sec
TD0 1

=====
CHANNEL f1
NUC1 1H
P1 10.10 usec
P2 20.20 usec
P12 3000.00 usec
PL0 120.00 dB
PL1 -2.00 dB
PL0W 0 W
PL1W 39.81071854 W
SFO1 600.1348010 MHz
SP1 41.43 dB
SPNAM1 Squal100.1000
SPOAL1 1.000
SPOFFS1 -1171.44 Hz

=====
GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 31.00 %
GPZ2 11.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 600.1313335 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



Compound S32

```
Current Data Parameters
NAME      TR4-133
EXPNO    13
PROCNO   1

F2 - Acquisition Parameters
Date_    20130402
Time     19.34
INSTRUM  av600
PROBHD   5 mm TBL5
PULPROG  mlevsgpph
TD       2048
SOLVENT  H2O+D2O
NS       2
DS       16
SWH      8389.262 Hz
FIDRES   4.096319 Hz
AQ       0.1221108 sec
RG       2298.8
DW       59.600 usec
DE       6.50 usec
TE       283.0 K
D0       0.00003316 sec
D1       1.00000000 sec
D9       0.06000000 sec
D12     0.00002000 sec
D16     0.00020000 sec
IN0     0.00011920 sec
L1      24

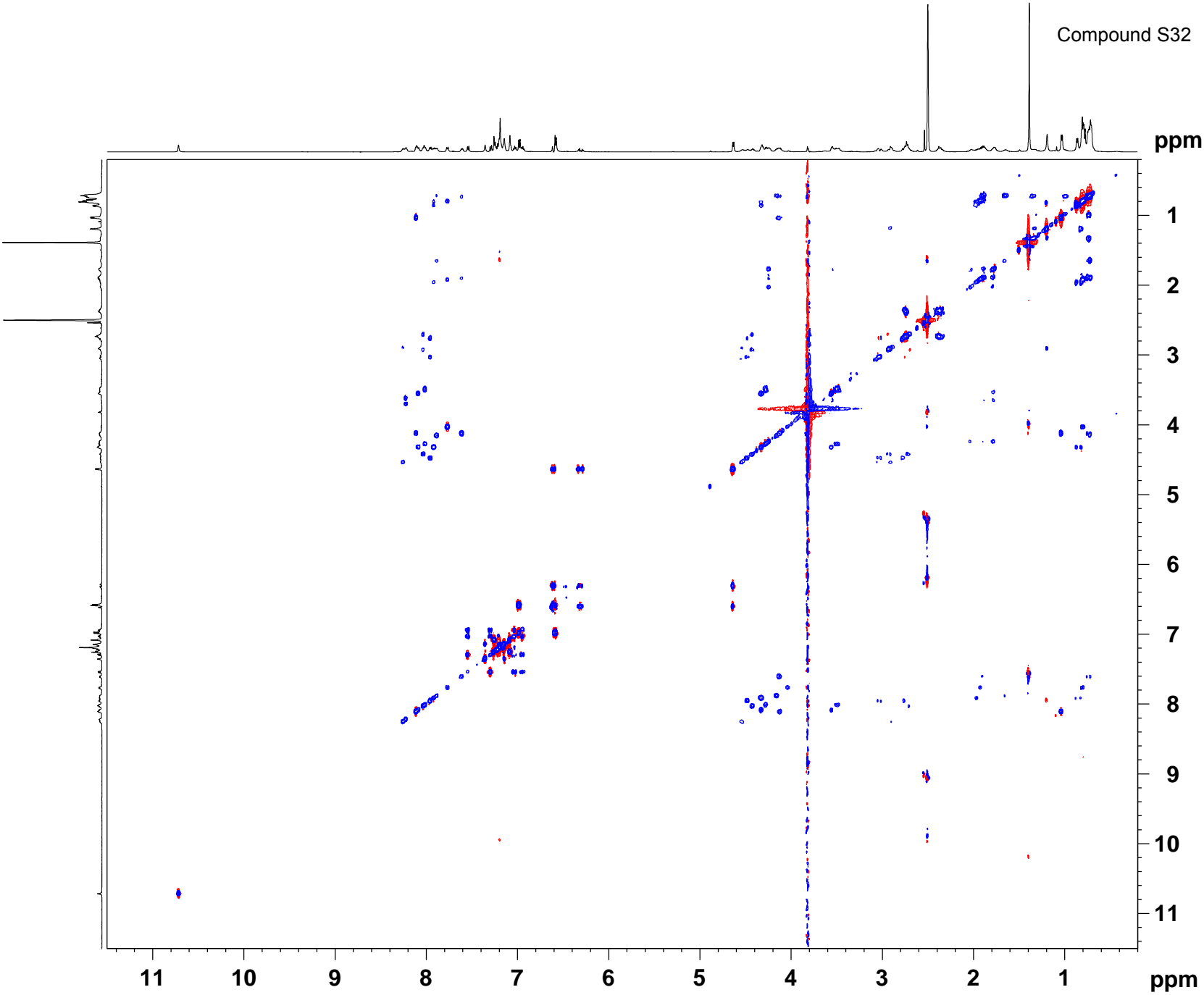
===== CHANNEL f1 =====
NUC1     1H
P1       10.12 usec
P2       20.24 usec
P5       26.68 usec
P6       40.00 usec
P7       80.00 usec
P12     3000.00 usec
P17     2500.00 usec
PL0     120.00 dB
PL1     -2.00 dB
PL10    9.94 dB
PLOW    0 W
PLLW    39.81071854 W
PLOW    2.54683042 W
SFO1    600.1348010 MHz
SP1     41.41 dB
SPNAM1  Squal100.1000
SPOAL1  1.000
SPOFFS1 -1175.04 Hz

===== GRADIENT CHANNEL =====
GPNAM1  SINE.100
GPNAM2  SINE.100
GPZ1    31.00 %
GPZ2    11.00 %
P16     1000.00 usec

F1 - Acquisition parameters
TD      256
SFO1    600.1348 MHz
FIDRES  32.770554 Hz
SW      13.979 ppm
FhMODE  States-TPPI

F2 - Processing parameters
SI      4096
SF      600.1313294 MHz
WDW     QSINE
SSB     3
PC      1.00

F1 - Processing parameters
SI      4096
MC2     States-TPPI
SF      600.1313325 MHz
WDW     QSINE
SSB     3
```



Compound S32

Current Data Parameters
NAME TR4-133
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130403
Time 18.54
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG noesyegpph
TD 4096
SOLVENT H2O+D2O
NS 8
DS 16
SWH 8389.262 Hz
FIDRES 2.048160 Hz
AQ 0.2441716 sec
RG 2298.8
DW 59.600 usec
DE 6.50 usec
TE 283.0 K
D0 0.00004674 sec
D1 2.00000000 sec
D8 0.30000001 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
INO 0.00011920 sec

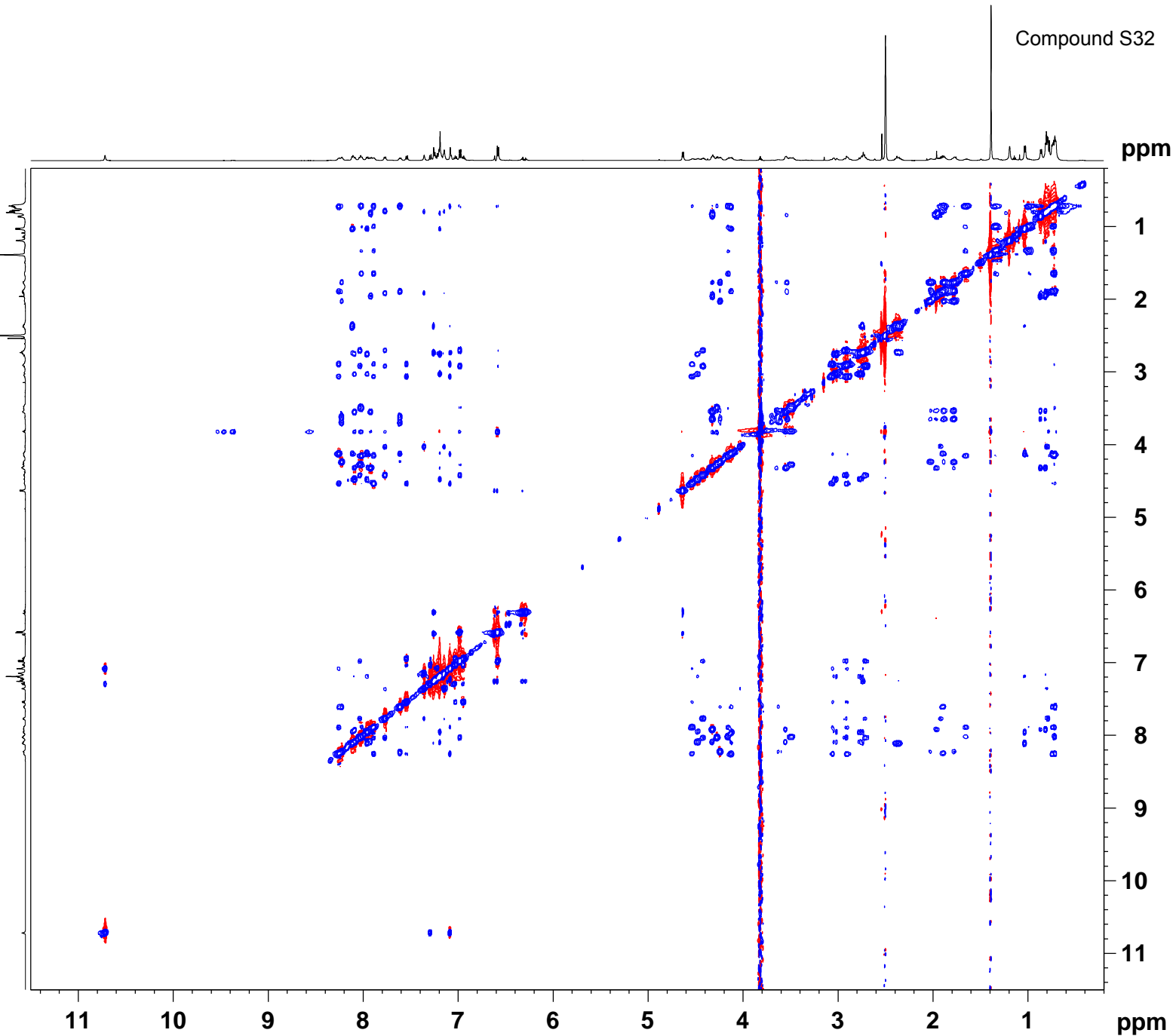
===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
P2 20.20 usec
P12 3000.00 usec
PL0 120.00 dB
PL1 -2.00 dB
PLOW 0 W
PLIW 39.81071854 W
SFO1 600.1348010 MHz
SP1 41.43 dB
SFOA1 Squal00.1000
SFOA11 1.000
SFOF1 -1171.44 Hz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 31.00 %
GPZ2 11.00 %
P16 1000.00 usec

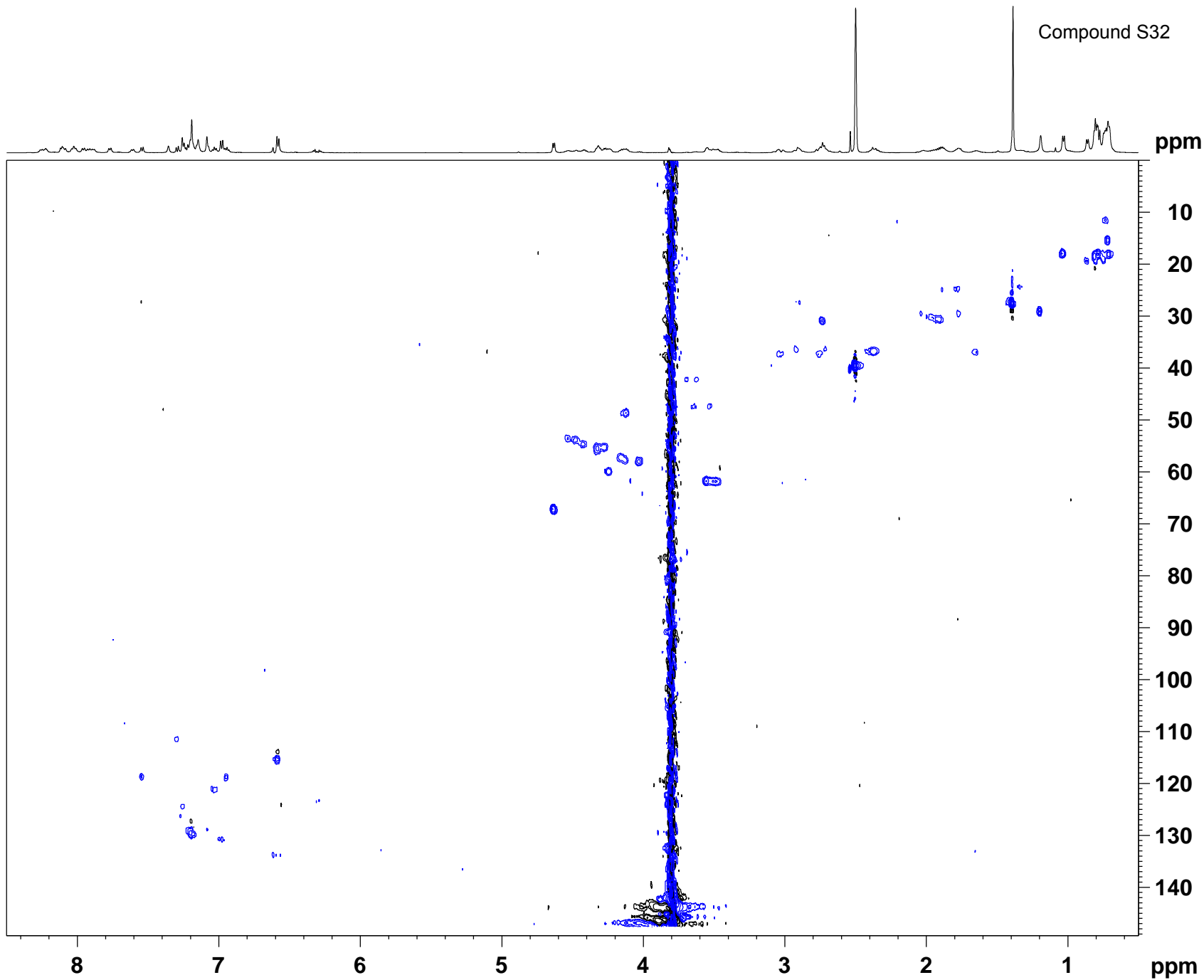
F1 - Acquisition parameters
TD 256
SFO1 600.1348 MHz
FIDRES 32.770527 Hz
SW 13.979 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 4096
SF 600.1313327 MHz
WDW QSINE
SSB 2
PC 1.00

F1 - Processing parameters
SI 4096
MC2 States-TPPI
SF 600.1313331 MHz
WDW
SSB 3



Compound S32



Current Data Parameters
NAME TR4-133
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130402
Time 19.58
INSTRUM av600
PROBHD 5 mm TBI5
PULPROG hsqcetspsisp
TD 2048
SOLVENT H2O-D2O
NS 8
DS -16
SWH 4921.260 Hz
FIDRES 2.402959 Hz
AQ 0.2081268 sec
RG 8192
DW 101.600 usec
DE 6.00 usec
TE 283.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086200 sec
IN0 0.00002070 sec
ZGPTNS

==== CHANNEL f1 =====
NUC1 1H
P1 10.12 usec
P2 20.24 usec
P2S 1000.00 usec
PL1 -2.00 dB
PL1W 39.81071854 W
SF01 600.1340570 MHz

==== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 19.52 usec
P4 39.04 usec
P14 1000.00 usec
PCPD2 65.00 usec
PL0 120.00 dB
PL2 -3.00 dB
PL12 7.45 dB
PLOW 0 W
PL2W 150.35617065 W
PL12W 13.55567932 W
SF02 150.9133722 MHz
SP3 4.12 dB
SPNAM3 Crp80,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz

==== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
F16 1000.00 usec

F1 - Acquisition parameters
TD 233
SF01 150.9134 MHz
FIDRES 103.631500 Hz
SW 160.000 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 4096
SF 600.1313291 MHz
WDW EM
LB 3.00 Hz
PC 1.40

F1 - Processing parameters
SI 4096
MC2 echo-antiecho
SF 150.9031666 MHz
WDW
SSB 2